Modeling the impact of fuel properties on compression ignition engine performance

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ABSTRACT OF THE
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Renewable fuels are of a great importance when aiming at decreased dependency from fossil resources in the transportation sector. This thesis, being part of ADVANCEFUEL project, encompasses examination of alternative fuels for light-duty engine purposes. Special attention is paid to the impact of fuel properties on modern compression ignition (CI) engine performance. The results are based on extensive literature review from publicly available sources. Interference between fuel properties and engine operating conditions is observed. Modeling is performed by multilinear regression method using data from driving cycles such as New European Driving Cycle (NEDC) and Worldwide harmonized Light vehicles Test Cycle (WLTC). Only representative, passenger car engine data is taken into account. Analyzed fuels and their blends with standard diesel are as follows: biodiesel (FAME), hydrotreated vegetable oil (HVO), biomass- or gas-to-liquid diesel (BTL/GTL). Density, lower heating value (LHV), viscosity, cetane number, oxygen and carbon content are selected as key fuel properties. The developed model predicts engine performance in terms of fuel consumption (FC) and CO_2 emissions from the end-user point of view. It enables to estimate a relative change of performance indicators in reference to standard fossil-based diesel. Based on literature sources, the maximum change of FC is +11,8% in case of pure FAME and -3,25% in case of HVO blends. The model satisfies theoretical values with good accuracy (average absolute error of 0,85% in FC). A promising potential in FC reduction is observed for high cetane number paraffinic diesel, including HVO. Finally, predictions of CO_2 emissions are based on outcomes from FC model and they indicate only tailpipe emissions changes.

Keywords: model development, system identification, alternative fuels, fuel blend properties, CI engine performance, fuel consumption, CO_2 emissions

Preface

In a foreword, I would like to warmly thank Professor Martti Larmi for his engagement, advice and support. He was the person who organized possibility for me to participate in ADVANCEFUEL EU project, part of Horizon 2020. The task was very challenging and required a lot of effort. However, shaping of the approach together with Yuri Kroyan and Martti Larmi was very exciting and teaching experience, especially in a Group of Thermodynamics and Combustion Technology at Aalto University. This thesis concluded my Joint Nordic Master's degree programme of Innovative Sustainable Energy Engineering studies. For the purpose of this work, I used relevant experience and knowledge from Bioenergy study track, comprising first year at KTH (Stockholm) and second year at Aalto University (Helsinki/Espoo).
Warm thanks to Ossi Kaario, especially for apt and valuable comments and advice during the project. Thanks to Thomas Kohl for taking part in ADVANCEFUEL project, too. I would like to also show my gratitude to Kai Zenger for his support in mathematical modeling. Moreover, I would like to thank Börje Kronström from St1 for his advice and organizing visit in refinery and meeting with Volvo R&D Team in Gothenburg. He arranged also web-conference with People from AVL Company. Also thanks to Teemu Sarjovaara for organizing meeting in Neste HQ and his contribution. Moreover, I would like to mention Mika Aho from St1, Daniel Danielsson and Sten Hovmark from AVL, Anders Röj and Per Hanarp from Volvo, and thank them for valuable advice.
Finally, I would like to express sincere gratitude to my family, especially my parents (Marek and Bogusia), brothers (Kuba and Wojtek) and grandmothers (Nana and Henia) for their support throughout the whole period of my Master thesis preparation and education. Their help made me finalize the work and endure all the difficulties. In the end, warm thanks to my colleague Yuri Kroyan for a great cooperation.

Otaniemi, 25.04.2018 Michal Wojcieszyk

Contents

Symbols and abbreviations

Abbreviations

AFR	Air-to-Fuel Ratio
AMF	Advanced Motor Fuels
ASTM	American Society of Testing and Materials
BDC	Bottom Dead Center
BMEP	Brake Mean Effective Pressure
BSFC	Brake Specific Fuel Consumption
BTE	Brake Thermal Efficiency
BTL	Biomass-to-Liquid fuel
CFD	Computational Fluid Dynamics
CFPP	Cold Filter Plugging Point
CI	Compression Ignition
CN	Cetane Number
CNG	Compressed Natural Gas
CR	Compression Ratio
CRI	Common Rail Injector
DF	Dual Fuel
DI	Direct Injection
DOC	Diesel Oxidizing Catalytic converter
DPF	Diesel Particulate Filter
ECU	Electronic Control Unit
E-FAME	Enzymatic biodiesel
EGR	Exhaust Gas Recirculation
EN	European Norm
EU	European Union
EUDC	Extra Urban Driving Cycle
FAME	Fatty Acid Methyl Ester
FC	Fuel Consumption
GHGs	Greenhouse Gases
GTL	Gas-to-Liquid fuel
Hck	Diesel with streams from hydrocracking process
HFO	Heavy Fuel Oil
HRR	Heat Release Rate
HVO	Hydrotreated Vegetable Oil
ICE	Internal Combustion Engine
IDI	Indirect Injection
IEA	International Energy Agency
IMEP	Indicated Mean Effective Pressure
ISO	International Organization for Standardization
LFL	Lower Flammability Limit
LFO	Light Fuel Oil
LHV	Lower Heating Value
LPG	Liquefied Petroleum Gas
LTC	Low Temperature Combustion
NEDC	New European Driving Cycle
NHA	Nozzle Holder Assembly
O2	Oxygen content [%m/m]
RDE	Real Driving Emissions

RME	Rapeseed Methyl Ester (rapeseed biodiesel)
SCR	Selective Catalytic Reduction
SI	Spark Ignition
STP	Standard Temperature and Pressure conditions
SVO	Straight Vegetable Oil
TDC	Top dead center
TWC	Three-Way Catalyst
UDC	Urban Driving Cycle
UFL	Upper Flammability Limit
UI	Unit Injector
WCO	Waste Cooking Oil
WLTC	Worldwide Harmonized Light Vehicles Test Cycle
WTW	Well-to-Wheel analysis

Symbols

b_e	Brake Specific Fuel Consumption
b	Bore
c_m	Mean piston speed
L_{st}	Air-to-fuel ratio
M	Brake torque
n	Rotational speed
p_e	Brake mean effective pressure
P_e	Brake power
s	Stroke
W_i	Indicated work
V_H	Engine displacement
η_e	Brake Thermal Efficiency
ϵ	Compression ratio
λ	Lambda value
ϕ	Equivalence ratio
ω	Angular velocity

Chemical compounds

CO_2	Carbon dioxide
DME	Dimethyl ether
H_2O	Water
HC	Hydrocarbons
NO_x	Nitrogen oxide
PAH	Polyaromatic hydrocarbons
PM	Particulate matter

1 Introduction

1.1 ADVANCEFUEL project

Figure 1: Partners of ADVANCEFUEL project [1].

ADVANCEFUEL project being part of the EU Horizon 2020 is a coordination and support action in response to the LCE 21 Call (European Commission Call for Low-Carbon-Energy) that focuses on targeted actions planned to provide clear and scientifically robust support for sustainable transport fuels. The purpose of the project is to facilitate the market roll-out of advanced liquid biofuels and other renewable fuels in the transportation sector between 2020 and 2030, with an outlook on post-2030 impacts. The goal should be achieved by providing the market stakeholders with state-of-art knowledge and sophisticated, user-friendly tools with integrated calculators, standards, and recommendations. Given knowledge and tools are going to support decision makers to remove the most prominent barriers against the commercialization of renewable fuels.

Figure 2: Main stakeholders of ADVANCEFUEL from Aalto Group [2], [3], [4], [5].

In order to accomplish the task, ADVANCEFUEL project was split into 8 specific objectives and 10 work packages. There are 8 partners working on the project and several stakeholders. Aalto is responsible for one of the objectives: *Recommend measures to increase market acceptance and end-use of renewable fuels based on a detailed market segmentation accounting for the role of fuel and fuel blend properties.*

This master thesis is related to objective O5 and work package WP5, which has the aim of improving evidence for market uptake. The purpose should be achieved by development of numerical tool in an open source format as a spreadsheet program. The tool is developed using mathematical models and methods based on the most relevant and recent knowledge obtained from publications in journals, conferences, workshops with end-use stakeholders and International Energy Agency (IEA). A research is conducted in the Group of Thermodynamics and Combustion Technology led by Professor Martti Larmi. The main activities of Aalto Group include Experimental Engine Combustion Research (low temperature combustion in dual fuel engines, alternative fuels and spray diagnostics, optical measurements on high pressure fuel injection and mixing) and Advanced Computational Energy Research (ignition and combustion characteristics in gas and dual fuel combustion, computational fluid dynamics (CFD) of chemically reacting flows and heat transfer). Despite the fact that data used for purposes of ADVANCEFUEL project are provided by external sources, the expertise and experience in the field are undoubtedly advantages while approaching the task of the project.

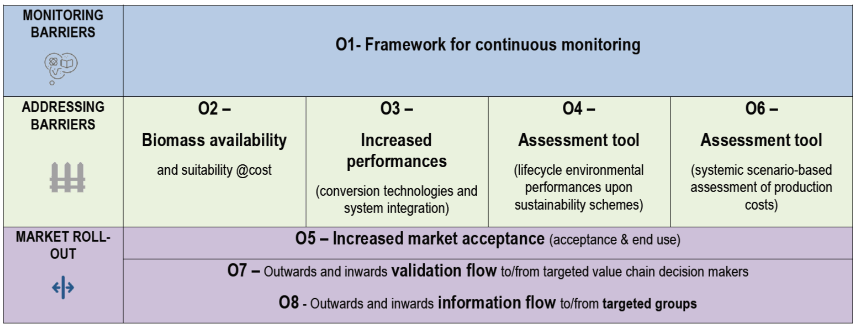


Figure 3: Division of objectives in ADVANCEFUEL project [1].

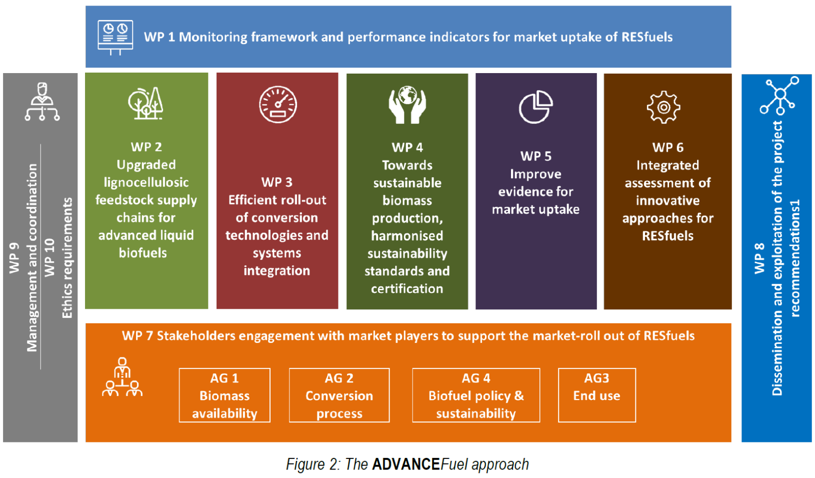


Figure 4: Division of work packages in ADVANCEFUEL project [1].

1.2 Motivation

Nowadays a lot of attention is paid to the CO_2 emissions and global climate change. At the beginning of 21st century policy makers and governments realized that stringent actions should be undertaken in order to prevent the natural environment and preserve our planet Earth in good condition for the future generations. However, strategic planning and intense actions should be performed in a confrontation with upcoming challenges of population growth followed by a sharp rise in energy demand. Currently, the global energy sector is mainly based on the fossil fuels, which are irreplaceable and limited in abundance. In addition, they are a tremendous source of CO_2 emissions into the atmosphere linked with the global temperature rise and eventually climate change. Total primary energy supply more than doubled in past 45 years, while fossil fuels including oil, coal and natural gas sum up to 82% of total fuel shares in 2015 [6]. When it comes to the total final consumption by sector, transportation is the second largest energy consumer with 29% shares in 2015 [6]. The significance of transportation in a modern world deserves a special attention, especially due to growing demand in developing countries. The current fleet of approximately 1 billion vehicles will be expanded up to 1.7 billion in next 20 years according to assumptions ([7] [8]). Moreover, a current status of fuels for transportation is dominated by the fossil oil products, which account for almost 95% of shares while biofuels approximately only for 2.5% [6]. Despite proved global oil reserves are estimated to cover demand for at least next 40 years [8], the world will eventually run out of fossil resources and alternatives will be required. Even more important, CO_2 emission reductions cannot be achieved without implementation of new technologies involving alternative fuels. Hence, there is a call for the market roll-out of renewable fuels, which will not only reduce emissions but also contribute to more sustainable global development and reinforcement of local economy or energy security.

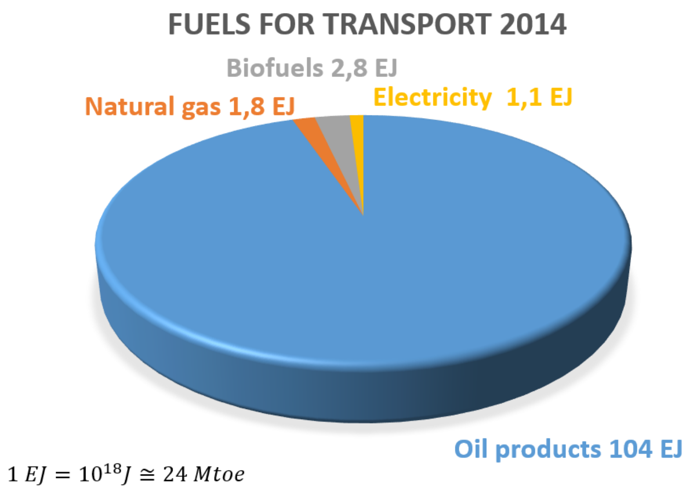


Figure 5: Fuels used globally in the transportation sector in 2014 - based on [9].

2 Scope of the thesis

This thesis is based on the research made during ADVANCEFUEL project. The main aim is to examine how fuel properties influence an engine performance. The task is specified for advanced biofuels used in CI engines. Moreover, the scope of this work encompasses only diesel engines for light duty sector. The investigation includes biofuels with a near-future potential of replacing some fraction of fossil-based diesel fuel. That is the reason behind considering in the initial stage of the project only drop-in fuels, which are compatible with current infrastructure and engine operation, including storage, refueling, injection and combustion characteristic. The outcomes of the thesis are based not on own laboratory experiments but on publicly available results from different researches around the world. Data necessary for modeling were collected from various literature sources such as recent journal publications (SAE, FUEL), databases (IEA AMF), conference papers or other projects. The complete schedule of the thesis with consequent steps is presented in Figure 6.

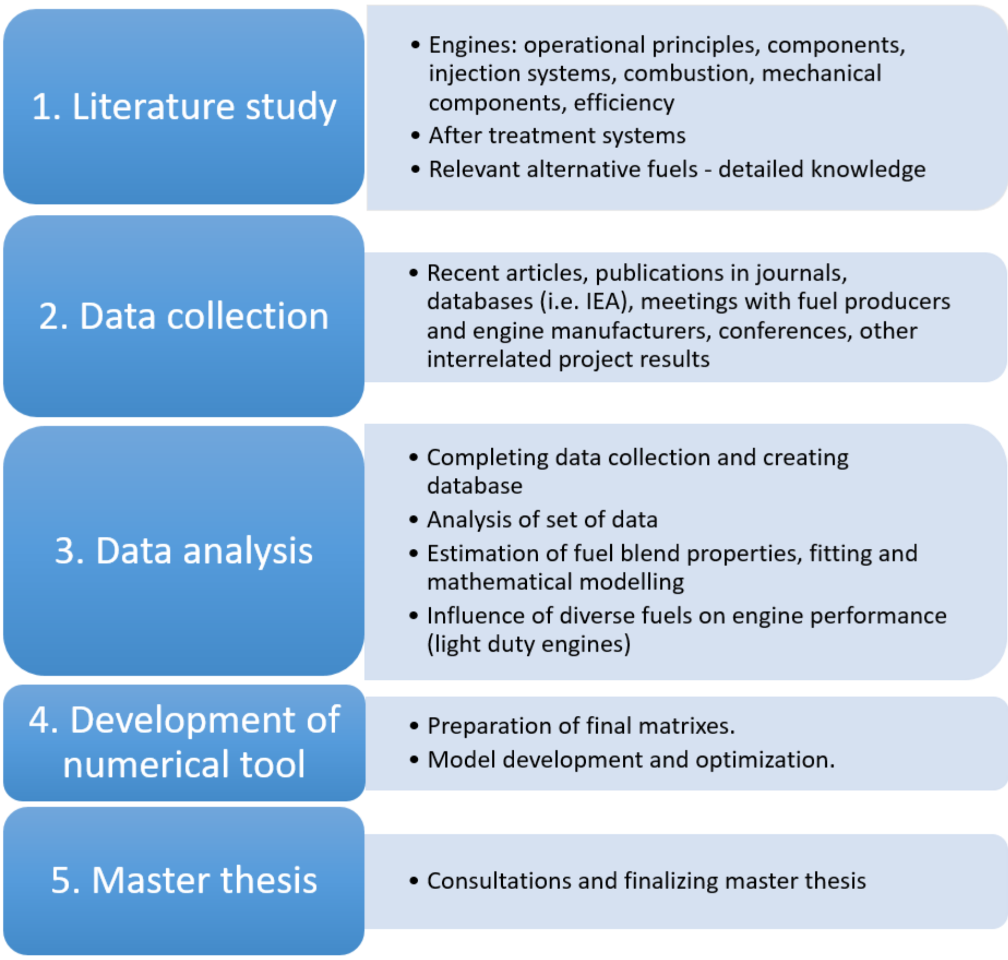


Figure 6: Subsequent steps to meet the final objective.

2.1 Work package 5 of ADVANCEFUEL project

The main goal of ADVANCEFUEL project is facilitating the market roll-out of alternative liquid fuels in transportation sector until 2030 and beyond. The actions within frameworks of the project include complete analysis for whole value chain of different biofuels. In order to properly assess the potential of alternative fuels, it is necessary to investigate complete WTW analysis. Hence, the whole work was divided into few packages in order to accomplish the final objective. This thesis is related to work package 5 (WP5), which has an aim of improving evidence for market uptake. WP5 is addressing objective 5 (O5) to recommend measures in order to increase market acceptance and end-use of alternative fuels based on a detailed market segmentation accounting for the role of fuel and fuel blend properties. Aalto University as a project member, which specializes in ICE, was responsible for the examination of fuel and fuel blend properties impact on end-use performance. The work initially was divided into different transportation modes including land, marine and aviation. Two parallel master theses were executed for the purpose of land transportation, especially light-duty engine types. This thesis written by Michal Wojcieszyk is related to CI engines, whereas second master thesis done by Yuri Kroyan encompasses SI engines. Both authors were closely cooperating during the project and two consecutive theses may contain the similar content in some parts. Worth mentioning is a fact that supervising Professor Martti Larmi together with both authors were shaping the project structure. That is why the approach in both theses is almost the same. However, in those works different fuels are considered, which influences unique specification of each thesis. Various transportation modes and exact part, which is covered by this thesis are presented in Figure 7.

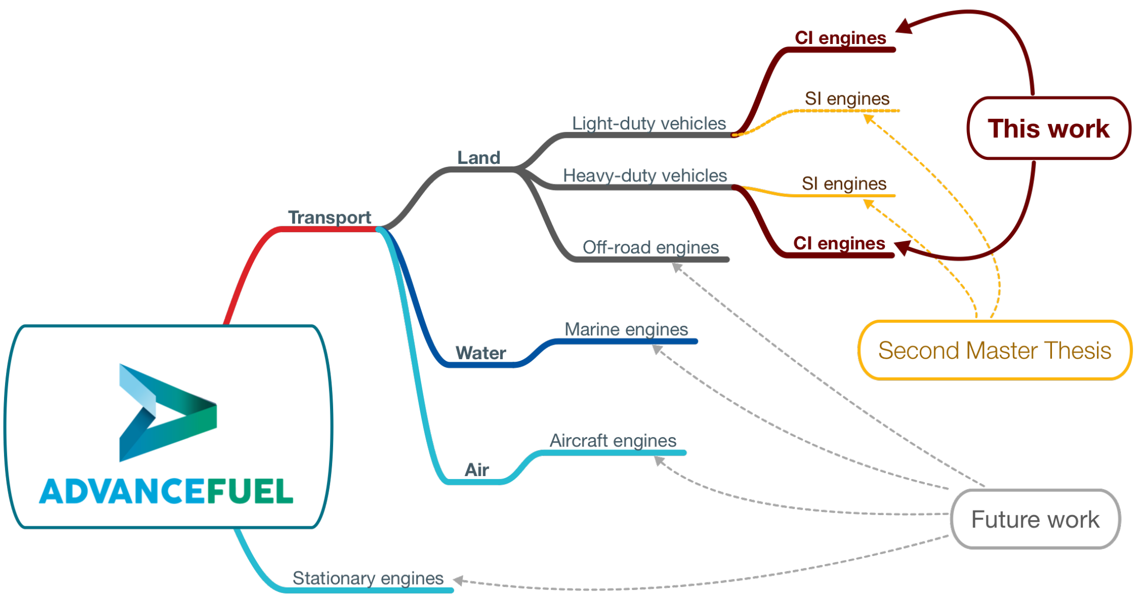


Figure 7: Division of WP5 in Aalto University.

3 Background

3.1 Engine and its performance

3.1.1 Compression ignition engines

Internal Combustion Engine

The subject of this work focuses mostly on the performance of a compression ignition (CI) engines used in transportation sector fueled by alternative liquid fuels and their blends with standard diesel. Before explaining CI engine (or sometimes called diesel-type engine) operation mechanisms, it is good to shortly mention about the heat engine, which is a broader classification and includes CI engine. The purpose of the heat engine is to produce useful heat from energy contained in the fuel in the form of chemical bonds. Useful heat is afterward converted into mechanical energy required for propulsion in the transportation sector. Among heat engines for the special attention deserve internal combustion engine (ICE) due to possibly compact overall size. In this type of engine burning or oxidizing of fuel proceeds inside the engine whereas air, fuel and burned gases are working fluids. In general, work transfers between those fluids and mechanical parts of the engine, provide the desired power output. In contrary, in external combustion engines, fuel is burnt outside the case of engine and it is powered by internal working fluid heated by an external source. Currently, there are plenty of types of ICEs available on the market. Design depends upon the final application, a condition of operation, fuel, etc. Some possible types of classification are presented in Figure 8. However, the main classification of ICEs with respect to this work is based on the method of ignition: spark ignition (SI) engines and compression ignition (CI) engines. Next important classification involves working cycle with the main distinction on four- and two-stroke cycles 3.1.2.

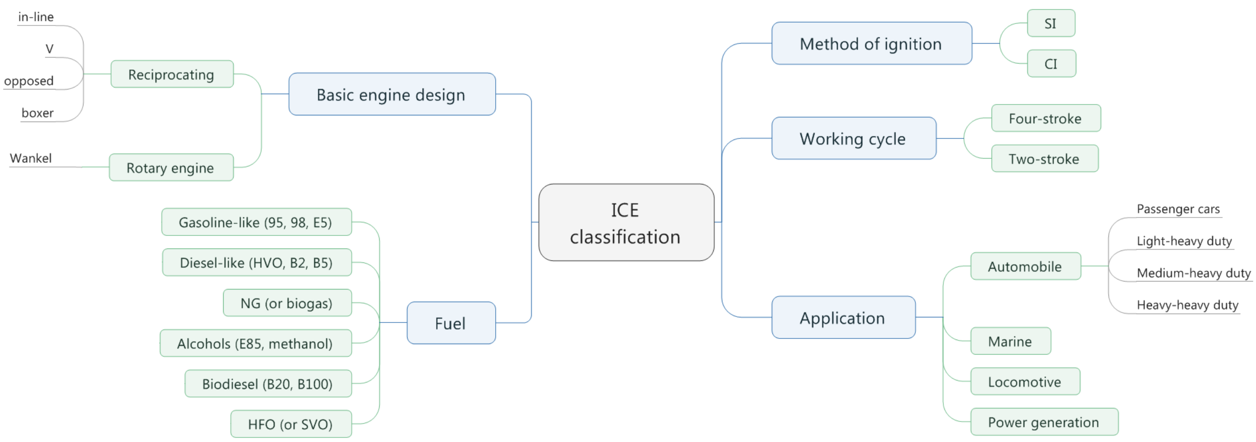


Figure 8: Classification of internal combustion engines.

Brief history of ICE

From the beginning of 19th century, Etienne Lenoir worked on the concept of a vehicle powered by gas, although it turned out to be unsuitable for driving machines. This was followed in 1870 by Nikolaus Otto's four-stroke engine concept, which is considered as a milestone in the development of ICE [10]. The engine was operated with liquid fuel and magneto ignition, but it was also characterized by poor efficiency. In 1897 Rudolf Diesel in cooperation with MAN (Maschinenfabrik Augsburg-Nürnberg) built the first CI engine based on his own concept. Acceptance tests proved the relatively high efficiency of a diesel engine in the given decade. However, the engine weighed 4.5 tones and that time it needed development to find a final application in a land use vehicle.

Design of ICE

Engines can be classified in respect to the basic design into two categories:

- **reciprocating** engines, in which the piston moves upwards and downwards in the cylinder,
- **rotary (Wankel type)** engine.

Nowadays almost all of the vehicles are run on reciprocating engines in different configurations (in-line, V, boxer) presented in Figure 9. The Wankel engine offers more compact design and better kinematics than a reciprocating engine. However, it did not gain significance due to drawbacks which prevailed over benefits. Main disadvantages of Wankel engine has an unfavorable design of combustion chamber and problems with sealing, which result in increased fuel consumption and pollutant formation [11].

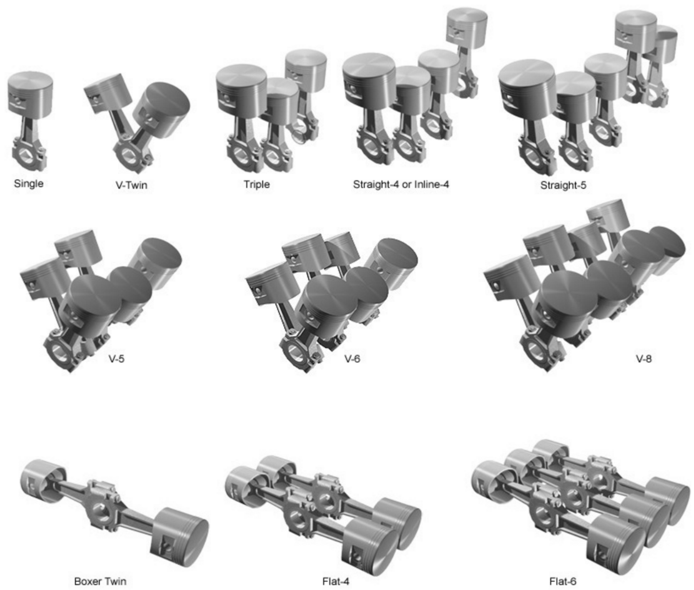


Figure 9: Different designs of reciprocating engines [12].

Two-stroke vs four-stroke engine

Nowadays the majority of engines in the transportation sector are vehicles operated on four-stroke cycle described in section 3.1.2. For the two-stroke cycle, there is one crankshaft revolution per power stroke in contrary to 2 revolutions for four-stroke mechanism. Two-stroke engines have some advantages over four-stroke ones. On the one hand, they can generate higher torque, have a higher power-to-weight ratio, are characterized by the easier lubrication, lighter flywheel and easier manufacturing process. On the other hand, four-stroke engines are more energy efficient, consume less fuel, generate less smoke and noise. Thus, fuel economy and emission restrictions support four-stroke engines used in transportation. Nevertheless, the most energy efficient ICE is a large two-stroke engine used for power generation and might reach thermal effective efficiency up to 54% [11].

Basics of operation and components

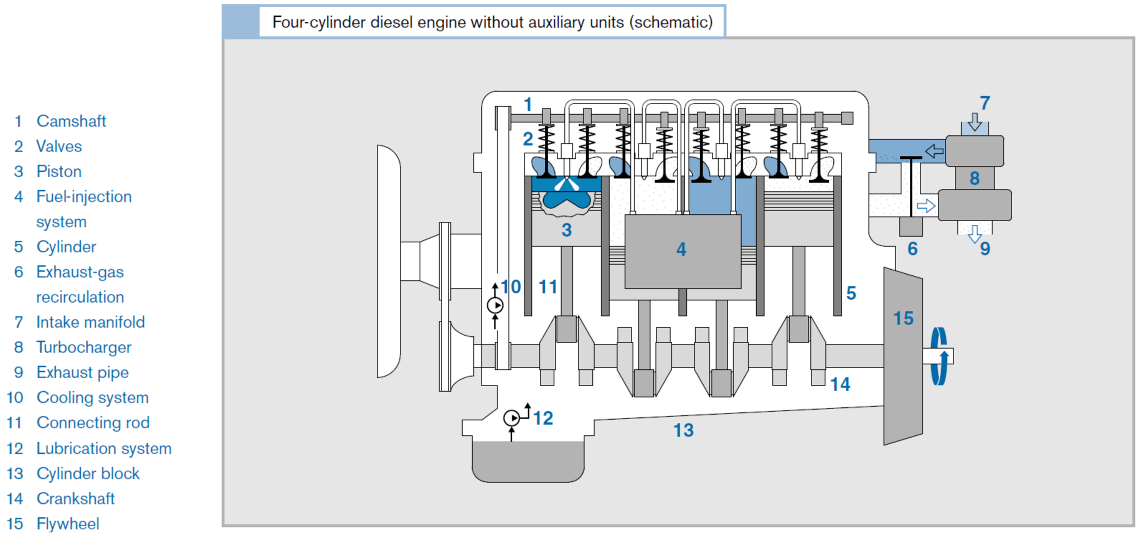


Figure 10: Standard diesel engine's components [13].

The diesel engine is ICE, which offers higher overall efficiency than SI engine. Beyond efficiency also associated with it lower fuel consumption made CI engines to gain such a huge share of the current automotive market. The diesel engine, in general, contains one or more cylinders. Inside each cylinder, there is a piston, which performs a reciprocating action. The whole process is driven by combustion of fuel in a combustion chamber inside the cylinder. The reciprocating movement is then converted into rotation of crankshaft connected to the piston by the connecting rod. A flywheel mounted at the end of the crankshaft is responsible for stable and continuous crankshaft rotation and also eliminates uneven rotation resulting from periodic nature of fuel combustion in separate cylinders. The crankshaft speed of rotation is associated with overall engine speed and usually is denoted in revolutions per minute.

Each cylinder is joined to the intake and exhaust valves, which respectively let the fresh air to get inside the chamber from the intake manifold and remove exhaust gases after combustion/expansion to the exhaust pipe. Those valves are automatically controlled by the rotation of the camshaft. Rotation of camshaft is intentionally coupled with the rotation of crankshaft in order to open valves in correct position of the piston. Another important part of the CI engine is an injection system, which provides fuel spraying into highly compressed air in the combustion chamber. Walls of the cylinders must be cooled and it is done by the cooling system. On the other hand, plenty of rotation elements, bearings requires suitable lubrication system. Worth mentioning is fact that modern diesel engines are turbo- or super-charged what improves efficiency and reduces emissions, as well as combustion noise. Exhaust gas recirculation (EGR) system is present in order to lower the NO_x emissions. The most important parts of CI engine are shown in Figure 10. In Figure 11 there are presented production materials and desired properties of those materials for different groups of engine components.

Property / Component	Density	Thermal expansion	Heat conductivity	Young's modulus	Ductility	Static strength	High cycle fatigue	Low cycle fatigue	High temperature strength	Wear resistance	Corrosion resistance	Property / Material
Crankshaft assembly components	(▽)			△	△	△	▲			△		Quenched and tempered steels and cast iron and aluminum alloys
Control components and injection equipment						▲	▲			▲		Hardenable steels, chill cast iron
Bolts					▲	▲	▲				△	Quenched and tempered steels
Supporting structures	▽	▽		△	△	△	▲					Cast iron and aluminum alloys
Hot parts		▽	△	▽	▲		▲	▲	▲		△	High and very high temperature strength alloys
Bearings					▲		▲			▲	▲	Laminated metallic composites
Radiators, coolers		▽	▲				△	△			▲	Aluminum copper and titanium alloys
Seals, filters, insulation			(▽)				△		△	▲		Special materials, elastomers and plastics

Symbols: ▲ high,required △ high,desirable ▽ low,desirable

Figure 11: Materials used for a construction of modern diesel engine [14].

3.1.2 Ideal and actual Diesel cycle

Ideal cycle

The concept of the Diesel engine was based on the ideal cycle for four-stroke engine presented in Figure 12 – ideal Diesel cycle. It consists of four consequent steps: intake, compression, power (ignition + expansion), exhaust and then the cycle repeats again from intake stroke. The Diesel cycle corresponds to idealized combustion in CI engines. Fuel is injected into the cylinder in higher pressure when compression is completed and ignition occurs without a spark.

The operation of CI engine can be described in accordance with the four-stroke mechanism. An intake stroke (0→1) starts when the position of the piston is in the top dead center (TDC), the fresh air is then drawn into the cylinder through the open intake valve from the manifold. The stroke ends when the piston reaches the bottom dead center (BDC) and the cylinder is filled with fresh air. During a compression stroke (1→2) all valves are closed and the air is compressed to the small fraction of its initial volume. The usual compression ratio ranges from 16 to 24 [13]. Towards the end of compression stroke, fuel is injected and combustion is initiated. A power stroke (2→4) starts from the TDC and piston is pushed by the high temperature and high pressure gases towards BDC. In this stroke, the power is delivered to run the engine while valves remain closed. An exhaust stroke (4→0) starts when the piston reaches BDC and exhaust valve is opened. This step ends while the piston is in the TDC position and chamber is scavenged from exhaust gases. Then the whole cycle repeats starting again from intake stroke. The four-stroke engine is characterized by the fact that the whole cycle requires 2 crankshaft revolutions.

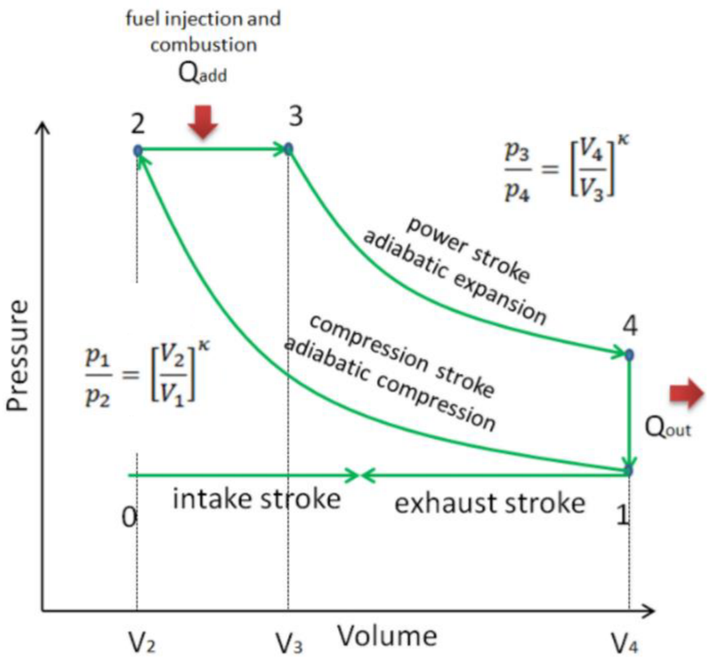


Figure 12: Ideal Diesel cycle on a pV diagram [15].

Actual cycle

Real cycle differs from the ideal one shown in Figure 12 and for better comparison example of the corresponding actual cycle can be presented in Figure 13. Variations from the ideal cycle occur because there are losses, which influence the shape of the cycle curve on *pV* diagram. Actual area restricted by this curve represents work delivered from one complete cycle and is always lower than for ideal cycle. The biggest difference is caused by the fact that fresh air replaces exhaust gases. So for an ideal cycle, there is a simplification in a manner of two horizontal lines ($1 \rightarrow 0$ and $0 \rightarrow 1$) representing exhaust and intake stroke respectively. In the actual cycle, there is a kind of loop called the gas exchange area, which should be also taken into account. Moreover, for the ideal cycle straight vertical line ($4 \rightarrow 1$) represents isochoric heat rejection whereas in the real cycle significant variation occurs as the cylinder chamber is scavenged from the exhaust gases. Another fact worth mentioning is an adiabatic process. In an adiabatic process, there is no heat transfer while in reality it cannot be fully reached. That is why for compression ($1 \rightarrow 2$) and power stroke expansion ($3 \rightarrow 4$) there are slight differences from the ideal case. Also, heat addition ($2 \rightarrow 3$) is not completely isobaric process. Next variation is related to the exhaust valve's early opening – blowdown losses might also appear. Moreover, the loss of maximum compression caused by the leakage of the gases through the piston rings may happen too.

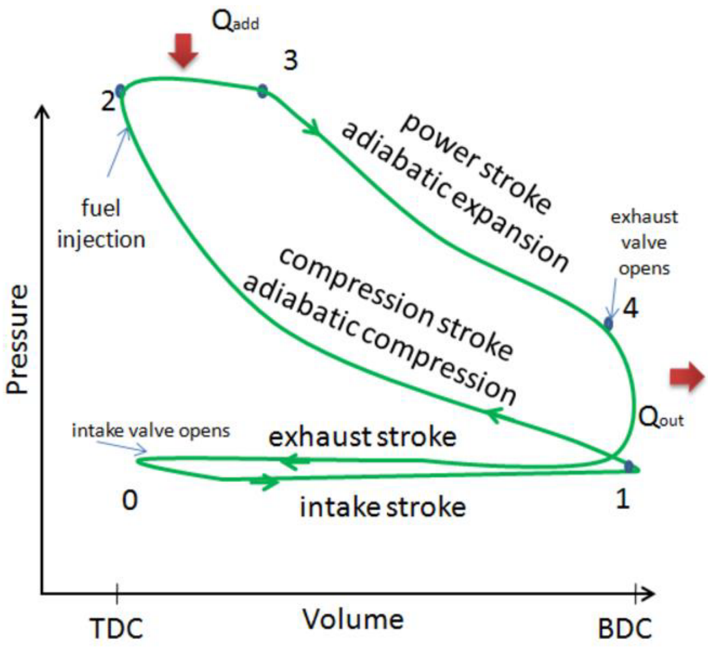


Figure 13: Real cycle in CI engine presented on *pV* diagram [15].

3.1.3 Engine efficiency

In a diesel engine, work delivered to the crankshaft is done by changes in pressure and volume of working fluids. Working gas is usually called as a cylinder charge. When comparing different designs, the term of effective engine efficiency is used. Effective efficiency contains all losses, starting from the thermal efficiency of ideal diesel process, through real process efficiency and finishing on fuel conversion and mechanical losses.

Thermal efficiency

Thermal efficiency denoted as η_{th} is an efficiency of an ideal Diesel cycle presented in Figure 12. The maximum theoretical efficiency of any heat engine operating between high temperature source and low temperature sink is set by the Carnot limit [16]:

$$\eta_C = 1 - \frac{T_{min}}{T_{max}} \tag{3.1.1}$$

Thus, the diesel thermal efficiency is always lower than for Carnot cycle. For an ideal diesel cycle, there are made some assumptions about the gas as a working fluid. It is assumed to be an ideal gas with constant specific heat. Flow losses during gas exchange are not considered. There are four main processes in the ideal diesel cycle. The first one is isentropic compression of fresh air. It means that no heat transfer occurs between working fluid and surrounding. The work is done on the working fluid. Isobaric heat addition is the second process – pressure is constant. The third one involves isentropic expansion. The work is done in this stage by the hot gases and again no heat transfer with surrounding appears. The fourth and last one is isochoric heat rejection – volume is constant.

Taking into account all above assumptions of ideal gas and ideal processes, thermal efficiency formula can be derived. Following the definition of thermal efficiency, it is the ratio of net work output (W) to the net heat input (Q_H) to the system [16]. Moreover, work can be presented as a difference between net heat input (Q_H) and net heat rejected from the system (Q_L).

$$\eta_{th} = \frac{W}{Q_H} = \frac{Q_H + Q_L}{Q_H} = 1 + \frac{Q_L}{Q_H} \tag{3.1.2}$$

Taking into account isobaric heat addition (Q_H) and isochoric heat rejection (Q_L), two equations can be written:

$$Q_H = mc_p(T_3 - T_2) \tag{3.1.3}$$

$$Q_L = mc_v(T_4 - T_1) \tag{3.1.4}$$

Inserting those two above equation into 3.1.2 results in the form:

$$\eta_{th} = 1 - \frac{T_4 - T_1}{\kappa(T_3 - T_2)} \tag{3.1.5}$$

Now using the adiabatic process relation ($pV^k - const$) and Clapeyron equation ($pV = nRT$) and rearranging 3.1.5, final thermal efficiency formula for Diesel cycle is obtained:

$$\eta_{th,Diesel} = 1 - \frac{1}{\epsilon^{(\kappa-1)}} \frac{\chi^{\kappa} - 1}{\kappa(\chi - 1)} \tag{3.1.6}$$

Concluding from the final equation, thermal efficiency is a function of compression ratio(ϵ), ratio of volume after and before the isobaric process (χ) and specific heat ratio of working fluid κ. (parameters in Section 3.1.4)
For the comparison, the ideal Otto cycle thermal efficiency associated with SI engine can be expressed as:

$$\eta_{th,Otto} = 1 - \frac{1}{\epsilon^{(\kappa-1)}} \tag{3.1.7}$$

Comparing both expressions for thermal efficiency, for the given compression ratio, Otto cycle has a higher yield. However, in a diesel engine, there is no risk of early autoignition and knocking problem is eliminated as only air is compressed. In practice diesel engine can be operated with significantly higher compression ratio. Moreover, there are lower pumping losses at part load as delivered power is controlled solely by injection system - in contrary to SI engine where this is controlled by throttling. That is why CI engine has actually higher efficiency than SI engine [17]. Typical compression ratio for SI engine is about 10 and for CI it is in range 16-24 [13]. Simulations for Diesel and Otto cycle are presented in Figure 14.

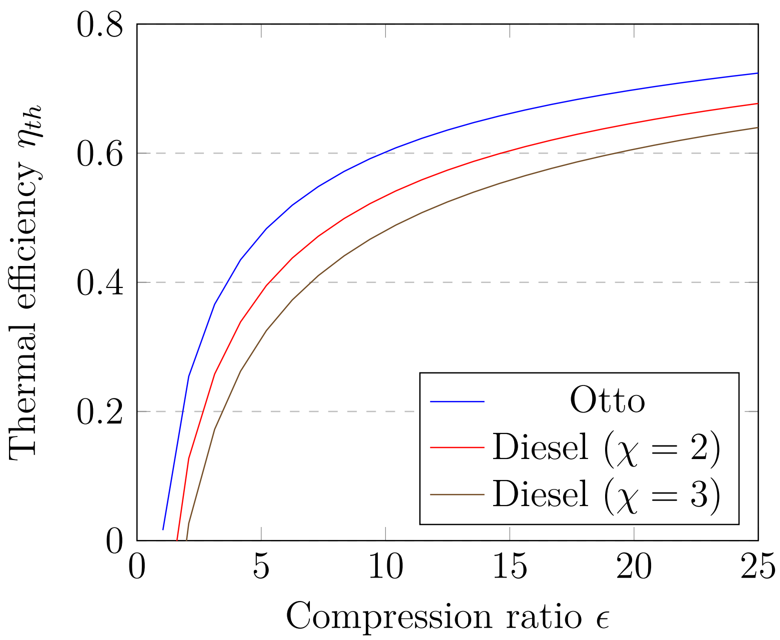


Figure 14: Comparison of thermal efficiency for ideal Diesel and Otto cycles. In consideration $\kappa = 1.4$. In reality, CI engine has better efficiency due to higher compression ratios and lack of throttling losses at part load.

The thermal efficiency of CI engine can be also derived from Seiliger cycle. It is another approximation of idealized process for diesel engines. All the previous cycle's subsequent steps remain the same as for diesel cycle but an extra process is added between adiabatic compression and isobaric heat addition. The added process is an isochoric heat addition (as the case for Otto cycle). The thermal efficiency of such a cycle can be expressed as presented in Equation 3.1.8 [18].

$$\eta_{th,Seiliger} = 1 - \frac{1}{\epsilon^{(\kappa-1)}} \frac{\tau\chi^{\kappa} - 1}{\kappa\tau(\chi - 1) + \tau - 1} \tag{3.1.8}$$

where τ is a ratio of pressure after and before heat addition process, respectively.

Cycle efficiency

Cycle efficiency (η_a) refers to actual cycle [13]. It is based on measured pressure and volume and includes deviations from the ideal cycle resulting from the usage of real working fluids instead of ideal gas. The finite speed of heat propagation is also taken into account during heat addition or rejection. The fully adiabatic process occurs only in theory and heat losses to the surrounding should not be neglected. In addition, significant difference results from considering flow losses during the gas exchange process – there is an extra pumping loop, which might also mean the work done during gas exchange by turbo- or supercharger.

Efficiency of fuel conversion

The efficiency of fuel conversion (η_b) informs about fuel inefficient combustion. Some part of energy contained in the fuel is not fully used, there are left some incomplete combustion products, i.e. soot, present in the exhaust gases and finally removed from the exhaust manifold. This is more related to the combustion system and uniform mixing of fuel with air.

Mechanical efficiency

Mechanical efficiency (η_m) includes different types of losses related to the moving parts of the engine. It encompasses frictional losses present at the piston, bearings and other assemblies and also aerodynamic and hydraulic losses in the crankshaft. When engine speed increases it entails higher frictional losses. At nominal speed, frictional losses might be split [13] as presented in Figure 15.

Brake thermal efficiency (BTE)

Brake thermal effective efficiency (η_e) of diesel engine informs about overall performance of the engine and is a composition of all previously discussed types of efficiency. It can be expressed as:

$$\eta_e = \eta_{th} \cdot \eta_a \cdot \eta_b \cdot \eta_m = \eta_i \cdot \eta_m \tag{3.1.9}$$

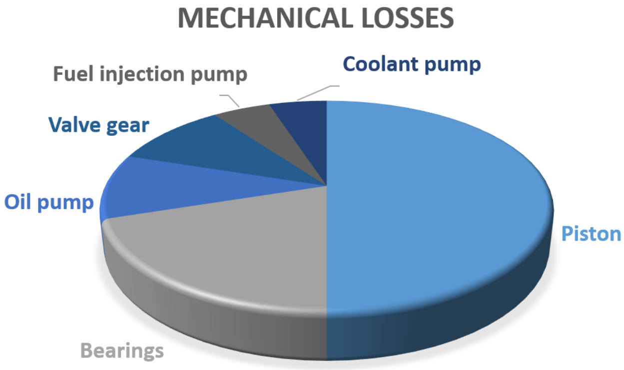


Figure 15: Mechanical losses in different parts of an engine. In the consideration, a supercharger is not taken into account.

η_i is an indicated efficiency and informs about **indicated work** (W_i) present at the piston referred to the energy contained in the fuel. Effective work available in the crankshaft is putting together indicated work available in the top of the piston and mechanical losses.
Another way to express the brake thermal effective efficiency is a comparison of effective power and available energy in the combusted fuel.

$$\eta_e = \frac{P_e}{\dot{m}_K \cdot H_u} \tag{3.1.10}$$

P_e - Brake (effective power)
m_K - Mass of fuel consumed per unit of time
H_u - Lower heating value of fuel

Brake specific fuel consumption (BSFC)

Effective specific fuel consumption (b_e) is very important measure inevitably related with the efficiency and it informs about fuel consumption in accordance to the delivered power. This parameter shows how efficiently an engine uses fuel in order to deliver power.

$$b_e = \frac{\dot{m}_K}{P_e} = \frac{1}{\eta_e \cdot H_u} \tag{3.1.11}$$

3.1.4 Engine parameters

For the engine designer and user, there are some important operational issues, which encompass engine's performance over its operation range, fuel economy, impact on local environment in the form of pollution, costs plus durability, reliability and future maintenance [18]. The current market design follows maximization of efficiency while decreasing environmental pollution. Engine designers without any doubt should

Engine type	BSFC $[g/kWh]$	Efficiency [%]
Small engines (two-stroke)	350	25
Motorcycle	270	32
Car SI	250	35
IDI diesel car	240	35
DI diesel car with turbocharger	200	42
Turbocharged truck diesel	190	45
Large diesel engine (two-stroke)	156	54

Table 1: Typical fuel consumption and maximum efficiency for different types of the engine [11].

take into account all those factors. Engine performance can be defined firstly by a satisfactory range of power and speed operation and secondly by the maximum power at different engine speed. Aiming at the comparison of different engine performances, very useful are parameters listed below [11].

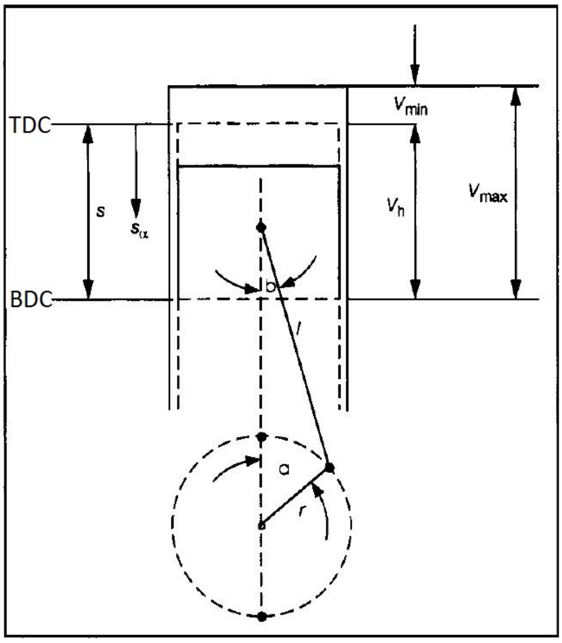


Figure 16: Sketch of the piston with parameters [11].

Piston displacement volume

Displacement volume of the piston (or swept volume) is the volume covered by the travel of the piston in the cylinder from the BDC up to TDC. The total displacement of the engine is a multiplication of single cylinder swept volume by the number of cylinders - Equation 3.1.12. In that way size of the engine is specified by the manufacturers. The size of the common diesel engines in passenger vehicles is around

2 liters.

$$V_H = V_h \cdot z = s \cdot \pi \cdot d^2/4 \cdot z \tag{3.1.12}$$

V_H - Volume of the total piston's displacement of the engine
V_h - Volume of the piston's displacement of the single cylinder
z - Number of engine's cylinders
s - Piston stroke
d - Cylinder bore (inner diameter)

Compression ratio

Compression ratio ϵ is the ratio between the maximum volume available for air when the piston is in the position of BDC and minimum volume (also called dead or clearance volume) when the piston is in the position of TDC.

$$\epsilon = \frac{V_{max}}{V_{min}} = \frac{V_h + V_c}{V_c} \tag{3.1.13}$$

V_c - Compression volume (or dead volume or clearance volume)

Rotational speed

Rotational speed n is a speed of revolving crankshaft and is specified by a number of revolutions in the given time, usually revolutions per minute (rpm).

$$n = \frac{number\ of\ crankshaft\ revolutions}{time} \tag{3.1.14}$$

Angular velocity

Angular velocity (ω) is a change of crank angle (α) in time during rotation of the crankshaft. This is directly connected with the rotational speed by the relation:

$$\omega = \frac{\partial \alpha}{\partial t} = 2 \cdot \pi \cdot n \tag{3.1.15}$$

Mean piston velocity

This parameter takes into account speed of reciprocating movement of the piston and is directly proportional to the rotational speed (n) and length of stroke (s).

$$c_m = 2 \cdot s \cdot n \tag{3.1.16}$$

When c_m increases, also inertia forces, wear and friction increase – that is why it might be increased only to some extent. As a consequence, large engines work at low/medium speeds and small ones can operate at higher speeds – rough correlation of mean piston velocity for a bore diameter in the range $0.1\ m\ < c_m < 1\ m$ can be approximated by Equation 3.1.17.

$$c_m = 8 \cdot d^{(-1/4)} \tag{3.1.17}$$

Mean brake power and torque

Brake power is a power available over the crankshaft of an engine. The power of an engine is calculated from the measured torque and angular velocity of the crankshaft (Equation 3.1.18). A dynamometer is a device for measuring the torque and hence brake power of an engine. Torque measured by dynamometer indicates the ability of an engine to do the work and power informs about the rate at which this work is done.

$$P_e = \omega \cdot M \tag{3.1.18}$$

Maximum rated power is the limit power that can be obtained from short, temporary engine operation. **Normal rated power** is the highest power allowed to be developed in the continuous operation of an engine. The distinction is made between continuous and temporary operation due to extensive wear and eventual destruction of the engine while operating in the maximum rated power for a diesel engine case. Rated speed is referred to the normal rated power and it describes the crankshaft rotational speed at which normal rated power is delivered.
Specific power output (P_l) and a **power-to-weight ratio** (m_G) are useful parameters when comparing an output of different engines.

$$P_l = \frac{P_e}{V_H} \tag{3.1.19}$$

$$m_G = \frac{m_M}{P_e} \tag{3.1.20}$$

Indicated work

Indicated work (W_i) per cycle can be calculated from an enclosed area in a Figure 13 and it represents energy transfer from gases to the piston. Net indicated work per cycle denotes work delivered to the piston over the whole four-stroke cycle and can be calculated from pressure and volume changes during the whole cycle making an integration.

$$W_i = \int p dV \tag{3.1.21}$$

Indicated work varies due to the intake system. In a case of naturally aspirated engines, pumping work transfer is to the gases as intake stroke pressure is lower than for exhaust stroke – negative work. In the case of turbo or supercharged engines, pumping work is transferred from gases to the piston – positive work. **Indicated power** can be presented as follows:

$$P_i = i \cdot n \cdot W_i \tag{3.1.22}$$

i - Working cycles per revolution;
$i = 1$ for two-stroke engine
$i = 0.5$ for four-stroke engine

Brake mean effective pressure

Brake mean effective pressure is a measure of the relative engine performance, not dependent on the size of the engine like in a case of brake power or torque. It is expressed by dividing an effective work by piston's displacement volume per cycle. Brake mean effective pressure is calculated usually from the brake torque (M).Thus, the performance of different size engines can be compared in that scope.

$$p_e = \frac{W_e}{V_H} = \frac{M \cdot 2\pi}{V_H \cdot i} \tag{3.1.23}$$

Engine type	Maximum speed $[rpm]$	Mean piston velocity $[m/s]$	Specific power output, max $[kW/l]$	Power-to-weight ratio, max $[kg/kW]$	Mean effective pressure $[bar]$
SI turbocharged car	7500	20	100	3	17
Diesel turbocharged car	5000	15	64	4	20
Diesel truck	4200	14	30	5.5	22
Medium speed diesel	1200	10	7.5	19	25

Table 2: Typical operational parameter's values for different types of engines [11].

Volumetric efficiency

Volumetric efficiency (λ_l) indicates the quantity of fresh air-fuel mixture (charge) in the cylinders at the end of an intake stroke. The more air-fuel mixture, the higher is a volumetric efficiency.

$$\lambda_l = \frac{m_Z}{m_{th}} = \frac{m_Z}{V_H \cdot \rho_{th}} \tag{3.1.24}$$

m_Z - actual charge mass in the engine's cylinders
m_{th} - theoretical charge mass
ρ_{th} - theoretical charge density

There are factors, which impact significantly volumetric efficiency such as fuel type and its heat of vaporization, temperature, compression ratio, the speed of an engine, a pressure in the inlet and exhaust manifolds, a design of intake and exhaust valves.

3.1.5 Engine operation

In the description of engine operation, it is important to determine, in which operational status the engine is currently running – start, no load, idle, full load, part load can be distinguished. Start of a diesel engine is a challenging issue and it requires cranking initiation, ignition and afterward action leading to self-sustained operation.

For the standard diesel fuel, minimum ignition temperature is around 250^oC. Such a temperature must be obtained irrespectively of unfavorable conditions – low ambient conditions, cold engine before the start or low speed of operation. Low outside temperature impact viscosity of engine oil what results in higher friction losses. In a cold weather also injection system may be affected because the viscosity of the fuel increases. The coldness of engine affects the heat losses through the combustion chamber surface. And a rule of thumb says that the lower an engine speed, the lower pressure and temperature rise is. Consequently taking into account all those three factors, some actions should be undertaken to avoid problems during cold start. One option is fuel heating prior to the injection system. The second solution involves start assistant systems, i.e. glow plug is mounted in order to assist temperature rise in the combustion chamber upon the start. The third option might be injection adaptation that entails injection of an excess amount of fuel and tailored injection timing in the starting phase. Next operational status is working under no load and it means that engine should overcome only its internal friction and no external useful torque is produced. The speed of the engine is unrestricted but during idle operation, it runs at the lowest speed. Another operational status refers to hard conditions of full load. In that case, the engine generates maximum possible torque and in the steady state condition, maximum allowed quantity of fuel is injected. A distinction between steady and non-steady state is based on the engine torque – if the produced torque equals required torque then it is steady state, otherwise, it is non-steady. The last status is part load, which is the medium state between full load and no load operation while torque is between zero and maximum value, too. The transition between operating states occurs when load or speed changes. It can be graphically presented on the engine characteristic maps.

For the diesel engine, the significantly higher compression ratio can be achieved as only air is compressed while for SI engine air/fuel mixture is susceptible to adverse knocking phenomenon. That is why in CI engine the air volume is kept constant while fuel quantity supplied is variable and it influences directly the power output of an engine. It is an advantage that there are significantly less pumping losses caused by no need of throttling as in a case of SI engine under instantly changing conditions. It is important to properly meter and distribute the fuel in order to comply with operation limits resulting from environmental issues. In that case, a key role is played by injection system which must supply the correct amount of fuel in a proper time and with appropriate pressure in accordance with instantaneous conditions. The operation of the engine should comply with emission restrictions, mainly PM and NO_x. The allowable pressure limit is established by the stresses throughout combustion chamber, which influences the durability and life-span of the whole engine. In addition, exhaust gas temperature should be kept below designed value in order not to destroy whole exhaust system. Recommended speed is also restricted by the stability of operation. The higher the speed, the higher friction present during operation and wear of construction material is deepened. Moreover, too high speed can lead to self-destruction. On the other hand, speed should not drop below the idle speed when no load is given. To keep the speed in the allowable range, the speed governor is installed. Finally, the engine operation is designed for the sea level pressure, so the injection should be adjusted for higher altitudes, too. The same applies to turbocharged engines.

Injection system

Injection in a diesel engine is a crucial process, which highly contributes to the combustion characteristics and consequently performance, fuel consumption, pollution and noise formation. Injection system consists of pumps, lines and injectors with nozzles. There are 4 main functions of the whole system: fuel delivery, high pressure generation, fuel metering and preparation. Fuel delivery is also called low pressure side and it means a transportation of fuel from the storage tank through a filter to the high pressure side. Generation of high pressure by a special pump is followed by delivery to metering point and requires valves to control the fuel mass flow. Fuel metering unit is responsible for a proper amount of fuel dosing and is obtained by piezoelectric or solenoid valves. Fuel preparation aims at optimal spray formation, distribution in the combustion chamber and it is achieved by the special design of nozzle and simultaneously by the interaction between nozzle needle and metering valve. Main parameters of injection are as follows: injection timing, pressure, quantity and rate of discharge. State-of-art engines use high injection pressure up to 2200 *bar* [13]. The electronic control unit (ECU) calculates injection parameters on the basis of the current operating status of an engine and ambient conditions. Different types of the injection system are presented in Table 3.

Injection system	**Short characteristic**
In-line pumps	separate pump element for each cylinder; plunger driven by the camshaft - reciprocating movement; fuel quantity controlled by the rotation of plunger governed by rack - an effective stroke of the plunger is variable, nozzle operation is pressure controlled
Unit injectors system	one unit injector per single cylinder; UI functions as a high pressure pump - thus pump and nozzle form one unit; UI is driven by the camshaft while high pressure is generated by the plunger; a nozzle is controlled by pressure; electronically controlled solenoid valve distribute proper amount of fuel and controls injection timing
Common rail system	accumulator injection system; the processes of pressure generation and fuel injection are separated; high pressure generated by one high pressure pump and then fuel accumulated in common rail - one line for all cylinders; injection controlled usually by piezoelectric valve with the use of electronic control unit; the nozzle is controlled by the lift; the amount of injected fuel and timing is a function of common rail pressure and an opening time of piezoelectric valve

Table 3: Different types of the injection system.

The injection nozzles are of the key importance in the injection system. They clearly influence mixture formation by proper distribution and atomization of fuel in combustion chamber. Moreover, they are the frontier between high pressure injection system and combustion chamber. Nozzles are a part of nozzle holder assemblies (NHA), unit injectors (UI) or common rail injectors (CRI) and are fixed in the cylinder head in a proper position. Their size is specified by the amount of injected fuel and cylinder displacement. Typical nozzle consists of nozzle body and needle. Needle opens during the start of injection and seals the injection system from the combustion chamber in a closed position. Nozzle holder assemblies and unit injectors are cam-driven and nozzle needle is pressure controlled. In a case of common rail, which contains fuel pressure accumulator, nozzle needle is controlled by the lift force, i.e hydraulic force [14]. Common designs of nozzles are pintle, hole type and nozzle modules. Pintle nozzles are used in IDI engines with NHA in older engines. However, modern diesel engines with DI operate with hole-type nozzles and nozzle modules. The main purpose of nozzle design aims at optimum conversion of high pressure into the high momentum of the spray in order to obtain the efficient spray penetration, break-up, atomization in conjunction with engine speed and load. Different types of the nozzle are presented in Figure 17.

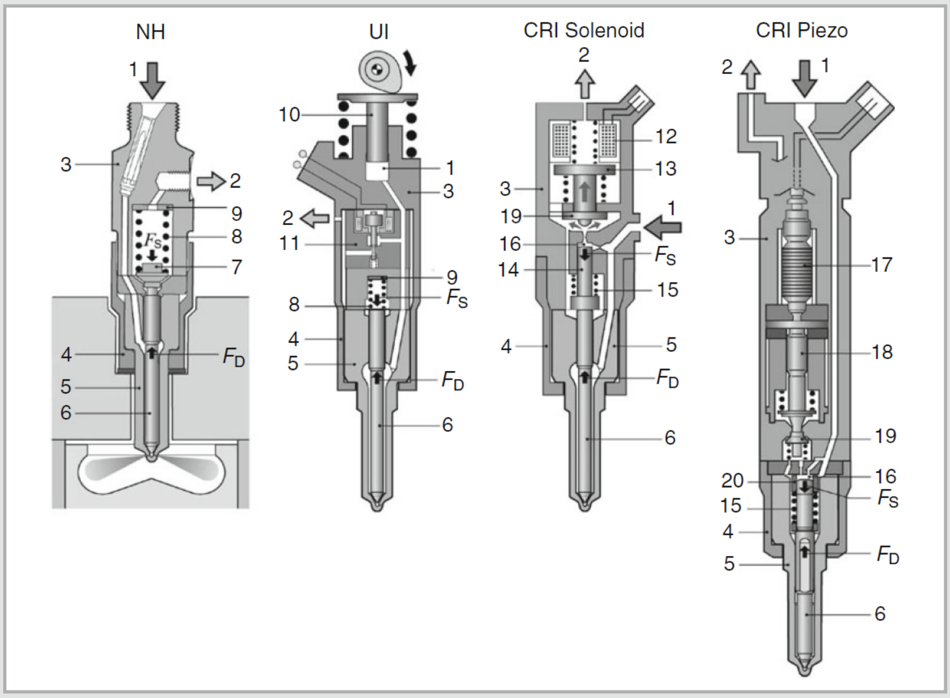


Fig. 5-3 Nozzle holders, injectors. *1* High pressure inlet; *2* Fuel return; *3* Nozzle holder; *4* Nozzle retaining nut; *5* Nozzle body; *6* Nozzle needle; *7* Thrust bolt; *8* Compression spring; *9* Adjusting shim; *10* Pump plunger; *11* Pressure control solenoid valve; *12* Solenoid coil; *13* Valve armature; *14* Push rod; *15* Return spring; *16* Control chamber; *17* Piezoelectric actuator; *18* Hydraulic coupler, *19* Control valve, *20* Control chamber sleeve

Figure 17: Commonly used injectors [14]. Modern engines tend to operate with piezoelectric injectors due to a very short time of response, which enables very precise injection timing.

Combustion chamber

Combustion chamber's shape and design are related to the injection system. Divided combustion chamber refers to indirect injection (IDI) and undivided one to direct injection (DI) system. Modern engines operate usually with DI due to better fuel economy – savings as high as 20%. Also, previous disadvantages of DI, such as noise and pollution formation, were in recent years overcome by the means of i.e. pre-injection process. Mixture formation in DI engine can be either controlled solely by fuel injection or assisted by intentionally forced air-flow turbulences. In the first case, wide and flat designs prevail and it is used for low or medium speed large engines with large piston displacement (i.e. marine engines). In the second case, deeper recess combustion chambers with significant swirl are preferred and it is utilized in passenger vehicles with high speed engines. The design of both cases is presented in Figure 18.

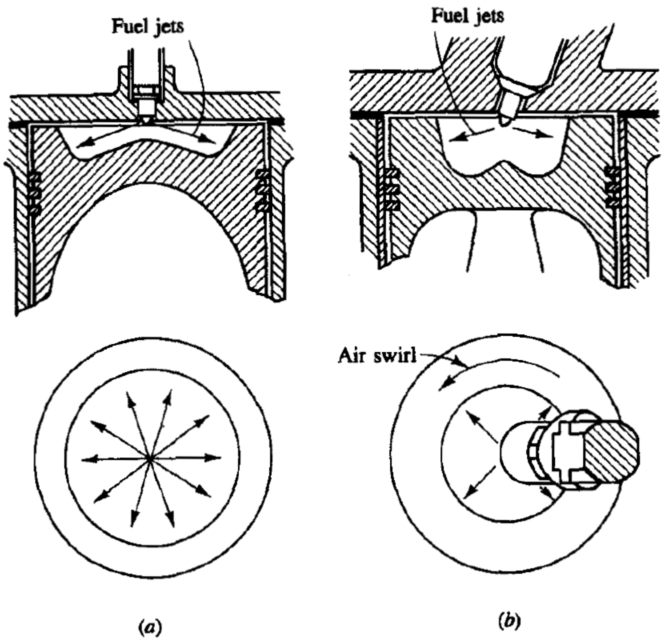


Figure 18: Comparison of combustion chambers in case of medium speed engine (a) and high speed engine (b) [18].

Cylinder charge control

Taking into account control of cylinder charge, engines can be divided into two groups:

- naturally aspirated,
- turbo/supercharged.

In naturally aspirated systems, the air is drawn into the cylinder under the atmospheric pressure. However, all modern designs deploy turbocharging. The distinction between turbo- and superchargers is based on the source of air compression in the intake duct. A **turbocharger** is run by the exhaust gases expelled from the cylinder after combustion. It consists of the turbine and coupled compressor and part of the exhaust gases' energy is recovered to drive a turbine. There are many designs including wastegate, variable geometry, variable sleeve or multistage turbocharging. Turbochargers are widely used in common vehicles in contrary to superchargers which are driven directly by the crankshaft. Utilization of waste energy contributes to the increased performance of an engine [13].

The whole charge control in recent concepts encompasses air filter, turbocharger (or supercharger), EGR and swirl flaps. Air filter eliminates dust and particles present in the intake air. This prevents from their entrainment in engine oil and wear in the bearings etc. In a case of lack of air filter, also airflow meter might be influenced by particle deposition. Mixture formation in the combustion chamber is influenced by fuel injection, the turbulence of airflow and movement of the piston. A whirl of airflow can be induced by the arrangement of intake ducts by the intentionally shaped swirl passage and by the fill channel with swirl flap. The aim is to reduce NO_x and particulate emissions.

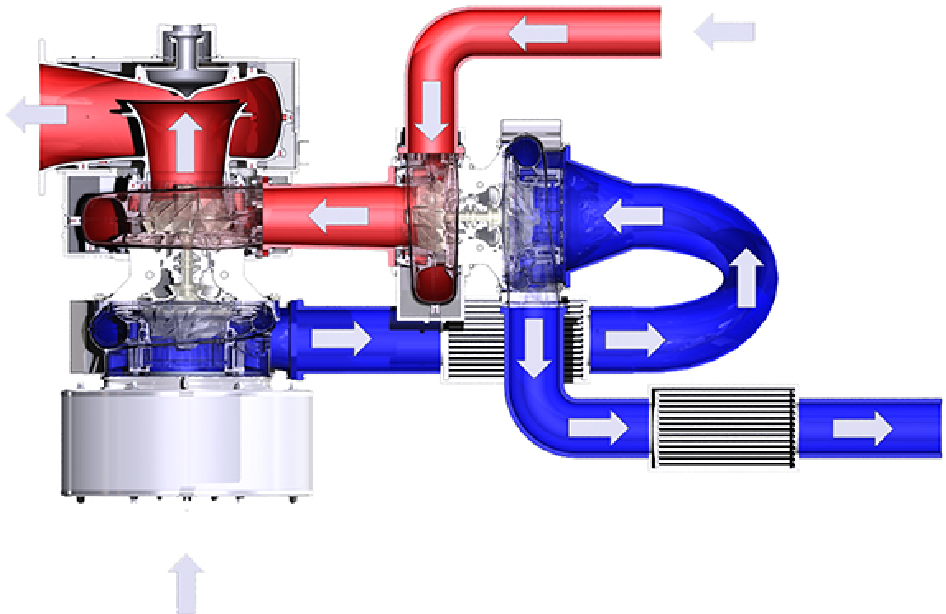


Figure 19: Two-stage turbocharger [19].

3.2 Combustion characteristics

The scope of this work focuses on alternative fuels and their blends with standard fuel used in CI engine. However, it is important to start from the description of traditional diesel fuel and its combustion characteristics. Basically, a fuel is any material that is altered in order to obtain useful energy in the form of heat or work. The release of energy is accomplished either by a chemical or nuclear reaction. The chemical reaction can be represented by the combustion mechanism. In principle, during combustion, an oxidant reacts rapidly with a fuel. Due to this reaction, the energy stored in the fuel is mainly released in the form of thermal energy, usually as hot gases. Beyond that, also some fractional amounts of electromagnetic energy (light), electric energy (free electrons, ions) and mechanical energy (noise) are produced [20]. The main oxidant used in the combustion process is oxygen because of its abundance in the Earth's atmosphere. Oxidation usually is conducted in the vapor phase except for oxidation of solid carbon – it takes place in the solid phase.

Conventional fuels are fossil-based, meaning that fuel is derived from the hydrocarbons (HC) deposits. This group encompasses coal, petroleum oil, natural gas. In past decades in the transportation sector, oil-based fuels took advantage over other types. For passenger cars, gasoline and diesel are used, meanwhile in marine light or heavy fuel oil and in aviation kerosene. All petroleum oil-derived fuels are processed in the crude oil refinement process. Refinement includes distillation while different fractions are collected based on the temperature of evaporation. Then processing such as cracking is done and blending of fractions is executed. Additives are put in the later stage. Starting from the lightest fraction: gases for chemical synthesis and CNG fuel, liquefied gases (for LPG), butane, gasoline, aviation/lighting kerosene, diesel, distillate and residual fuel oils (HFO, LFO), lubricating oils, paraffin oils and waxes.

Complete combustion of HC refers to the final condition that all carbon and hydrogen atoms of the fuel are gathered in the form of carbon dioxide (CO_2) and water (H_2O) in the flue gases. A stoichiometric reaction is a reaction in which the exact amount of oxygen is supplied in order to perform complete combustion. The laws underlying stoichiometric combustion are as follows: elementary reaction equation, element and mass conservation. In theory, reactants after combustion in the stoichiometric reaction should be fully oxidized after supplying exact amount of oxygen. Nevertheless, in reality, excess air is required to obtain a state of complete combustion. Stoichiometric **air-to-fuel ratio** (L_{st}) is a measure of air fed to the system. It denotes how many kilograms of air is necessary to complete burn 1 kilogram of fuel (in theory).

$$L_{st} = \frac{m_{L,St}}{m_K} \tag{3.2.1}$$

$m_{L,St}$ - Air mass under stoichiometric conditions
m_K - Fuel mass

Actual air-to-fuel ratio informs about real amount of oxygen brought to the system. The ratio between actual and stoichiometric air-to-fuel ratio is denoted as **lambda** (λ).

$$\lambda = \frac{m_L}{m_{L,St}} = \frac{m_L}{m_K \cdot L_{St}} \tag{3.2.2}$$

m_L - Actual air mass

Another measure of excess air might be **equivalence ratio** (ϕ), which is a ratio between a stoichiometric mass of oxidizer and actual one in the system.
Incomplete combustion leads to the state, in which flue gas contains also combustible elements. Those molecules can be further oxidized with a release of energy. That is why some part of fuel energy is lost during incomplete combustion. There are specific conditions, which promote incomplete combustion, mainly insufficient air supply, too short residence time of fuel in the combustion zone, low mixing of air/fuel, and too low temperature.

Fuel combustion rate, which informs about the speed of reaction, is specified by three main factors [20]:

- a rate of chemical reaction between fuel and oxygen depended from the used fuel and its components,
- a rate of oxygen supply to the reaction zone during combustion,
- temperature prevailing in the combustion zone.

Forced action like raised temperature or turbulence caused by mixing, can increase the fuel combustion rate. Classification of fuels is based on its physical state. Different states of fuels influence the equipment necessary for combustion. Fuels covered in this paper are only in liquid phase. Fuels are chosen based on its availability, easiness of usage, economy and susceptibility to emissions.

3.2.1 Diesel engine combustion

For CI engines, combustion is controlled by turbulent mixing. The combustion process in a diesel engine is directly influencing the overall performance, fuel consumption, emissions formation and noise pollution. Its characteristics are directly connected with the fuel properties. In diesel combustion, knocking, as in the case of SI engines, is eliminated due to fact that only air is compressed and therefore operation can be conducted with greatly higher compression ratios. A pressure in current designs can reach $180 - 230$ *bar* in the cylinder [14]. As a consequence, CI engine is characterized not only by improved efficiency but also by better torque performance. The combustion process in the diesel engine can be divided into three consequent steps, namely mixture formation, ignition and proper combustion. In contrary to spark ignition, in compression ignition engine fuel is injected under very high pressure (up to 2200 *bar* [13]) and it refers to internal mixture formation. Then the heat is transferred from the hot compressed air to the fuel which auto-ignites. That is the reason for the demand of highly ignitable fuels classified by high cetane number. Finally, proper combustion proceeds and fuel energy is released in the form of heat. In this stage, expansion of stroke is executed and also pollutants are formed.

3.2.2 Mixture formation

Advanced diesel engines operate with direct injection system and lambda value in a range from 1.2 (in full load) to 7 (in a case of idle status) [11]. Thus, the mixture is heterogeneous and its formation is dominated by the injection system. The most important factor influencing adequate mixture formation is a **momentum of the fuel spray**. The key parameters are the quantity of injected fuel, time and pattern of injection, pressure gradient in the injection nozzle and geometry of the nozzle. Hence nozzle together with injector design plays a key role influencing whole diesel combustion. The spray energy is determined by the delivery rate of injection pump for cam-regulated injection and rail pressure for a common rail system. The injection pressure ought to increase or at least remain constant in time during the injection process. Spray penetration is required to be immediate as for the direct injection the mixture formation lasts only a few milliseconds. Fuel spray in a properly designed combustion system should not hit the walls of the combustion chamber. During penetration spray break-up occurs and surface area of fuel is multiplied. In a primary break-up, there are different forces working on the fuel spray. It encompasses viscosity, surface tension, aerodynamic forces, turbulence and cavitation produced in the nozzle by highly turbulent fuel flow. Also temperature and fuel composition and volatility influence spray break-up. In a secondary break-up, the spray is atomized meaning that small microdroplets are formed. Here, the aerodynamic forces play a key role. If the injection pressure rises, it is followed by the finer droplet formation and in consequence, more air reaches the spray. Air density in the chamber also should not be neglected. Airflow in the combustion chamber plays also an important role. Air swirl is generated intentionally by means of the design of combustion chamber and intake port. Its purpose is to break up the compact fuel spray into smaller droplets and mix them with the air [14]. The air swirl increases with the engine speed because of the piston movement. However, too high swirl can lead to significant wall heat losses as well as its generation impact charge losses. The solution may be with helical ports, which enable almost linear increase of air swirl with engine speed. In that case, some kind of trade-off between necessary swirl and volumetric efficiency can be achieved. Swirl is increased during the compression stroke when the air is squished into the piston crown. The squish influences the mixture formation while momentum is exchanged between air and fuel. A proper design of the piston bowl allow forming turbulent flow and therefore helps mixture formation and rate of combustion.
After breakup, evaporation process occurs and is driven by the heat transfer between hot compressed air and fuel spray. The higher injection pressure and smaller fuel droplets, the faster evaporation of the fuel. Reaction and diffusion zones can be distinguished. Lambda value changes across the mixture from 8 away from droplet till 0 in the center of the droplet. Overall lambda in a flame region ranges from 0.3 to 1.5 [14]. However, lambda in a combustion zone, where heat is released, oscillates

around a value of 1.

3.2.3 Ignition and heat release

Fuel is injected before the piston reaches TDC as there is present ignition delay. This is a time between a start of injection and start of ignition. It results from the previously discussed break-up and evaporation (physical ignition) and additionally from the reaction rate while ignition radicals are initiated (chemical ignition). The fuel itself and its susceptibility to auto-ignition is a crucial factor determining the easiness of start of ignition. The longer ignition delay might result in elevated noise formation. In modern diesel engines ignition delay lasts as short as $0.3 - 0.8\ ms$ [14]. The injection pattern and timing allows controlling the combustion and final energy conversion. There is a need for a rapid energy conversion in order to avoid undesired heat losses and pollution formation. On the one hand, the longer ignition delay, the lower rate of soot formation. On the other hand, the shorter ignition delay, less NO_x and unburned HC are produced. Also, combustion noise is negatively influenced by the longer ignition delay. In addition, energy efficiency must be compromised with restrictions of exhaust emissions.

3.2.4 Pollution formation

In a diesel engine, a heterogeneous inner mixture is formed, what means that there is a gradient in lambda value inside the combustion chamber. This charge stratification results in the formation of pollutants in different regions of the fuel-air mixture. Main pollutants which emissions are regulated and restricted by law are: NO_x, particles (PM), HC and CO. They are present in the exhaust fumes and their qualitative formation is shown in Figure 20. NO_x formation is inevitable in lean zones with very high temperatures at an outer part of the spray droplet. Nitrogen oxides, NO and NO_2, are mainly thermally formed at the flame front. For diesel engine, the ratio of NO-to-NO_2 is in the range 0.6-0.9 [11]. Excess air and elevated temperature are factors, which positively contribute to the NO_x formation. Unburned HC and CO are formed in the outer lean zone with lower temperature. In this lean region outside the flame zone, the oxygen concentration is too low to fully oxidize HC. Injection system and mixture formation play a key role, thus post-injection can cause higher HC emissions. However, their concentration is considerably lower than for SI engines. Particles formation occurs in a rich region inside the spray core. Those are mainly HC particles, which can finally form soot, the remaining small fraction might be sulfates in a form of aerosols. The reaction of formation PM is started by free radicals, then PAH are formed by polymerization and eventually compounds aggregate, creating larger PM. Another contributor to PM formation may be lubricant combustion. The creation of PM is influenced mostly by local temperature and oxygen concentration. The pollutant formation is also connected with the temperature profile, which is characterized by low temperature inside the droplet and the highest possible temperature is in the lean region of $\lambda = 1.1$ reaching over $2000K$ [14]. The ultimate air exploitation in the combustion chamber is

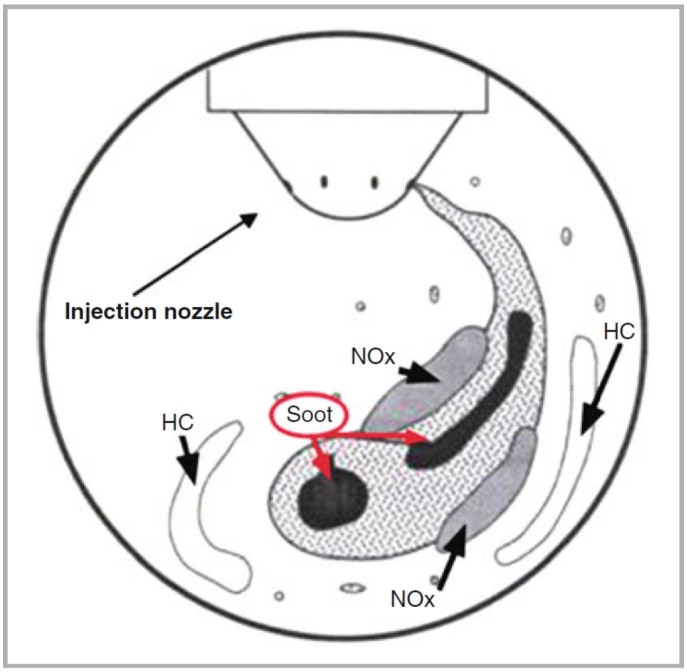


Figure 20: Qualitative presentation of pollutants formation in diesel engine [14], [11].

not feasible and excess air supply is demanded. Due to that fact, three-way catalyst (TWC) operating without excess air used in SI engine, cannot be installed in a diesel aftertreatment system. Thus, it is required for deployment of other technologies such as oxidation catalytic converter for HC, CO or EGR, SCR for NO_x or DPF for PM. Besides the restricted pollutants, certainly CO_2 emissions should be mentioned - they are significantly lower than for SI engines, even up to 20%.

A particular problem with pollutant formation in diesel engine encompasses conflict between favorable conditions for PM and NO_x formation. On the one hand, elevated temperature eliminates a problem with soot formation. On the other hand, the higher is a temperature, the more NO_x is formed. The same situation is for lambada value. The more excess air in the combustion chamber, the less soot is formed. Nevertheless, it is also followed by increased NO_x emissions. Those relations between soot and NO_x formation dependent on temperature and lambda value are presented on a $\phi - T$ map in Figure 21. Concluding from the above considerations, some trade-off must be done while designing the combustion system. Finally, that is an additional reason, why the extra aftertreatment system must be included to comply with emission regulations.

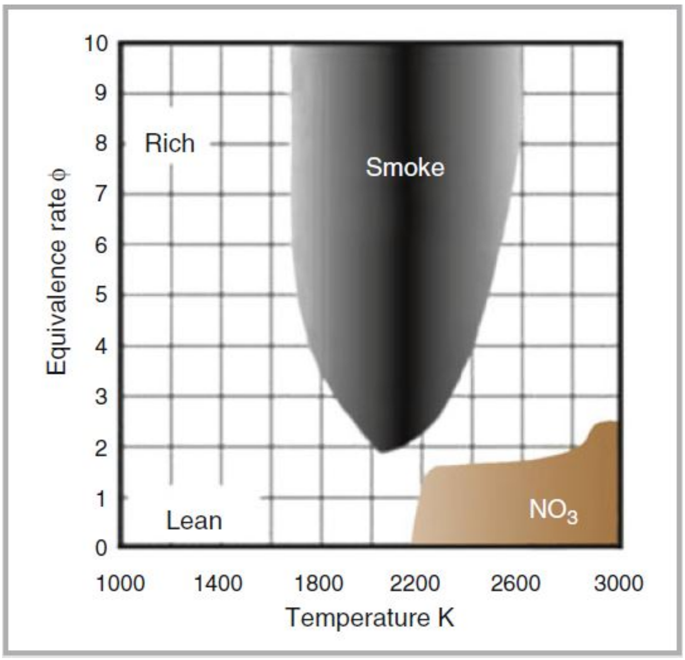


Figure 21: $\phi - T$ map showing an influence of air/fuel mixture composition on the PM and NO_x formation [14].

Specific emissions

Specific emissions parameter (s_i) informs about the mass of specific constituent of the exhaust gas produced per delivered power of an engine.

$$s_i = \frac{m_i}{P_{out}} \tag{3.2.3}$$

i is a component such as NO_x, CO, unburned HC etc...

3.3 Fuel characteristics

3.3.1 Fuel standards

Fuel owns many important properties, which influence combustion in a diesel engine, thus its overall performance. In order to ensure reliable operation of an engine in the transportation sector, there was a need for standardization as in a case of diesel fuel. ASTM establishes diesel fuel requirements in the US while it is a role of European Committee for Standardization (CEN) in the European Countries. EN 590 is a standard approved by CEN and all member countries must comply with it. In the EN590 standard, restrictions and minimum requirements of diesel fuel are precisely described and measurement methods of International Organization for Standardization (ISO) are listed. Below, table with detailed requirements of EN 590 standard and detailed description of each property. For FAME biodiesel there is another standard EN 14214, whereas paraffinic fuels have their own specification - EN 15940.

Property	Unit	Limits		Test method [a]
		minimum	maximum	(See 2. Normative references)
Cetane number [b]		**51,0**	–	EN ISO 5165 EN 15195
Cetane index		46,0	–	EN ISO 4264
Density at 15 °C [c]	**kg/m^3**	820,0	**845,0**	EN ISO 3675 EN ISO 12185
Polycyclic aromatic hydrocarbons [d]	**% (*m/m*)**	–	**11**	EN 12916
Sulfur content [e]	**mg/kg**	–	**50,0** until 2008-12-31	EN ISO 20846 EN ISO 20847 EN ISO 20884
			10,0	EN ISO 20846 EN ISO 20884
Flash point	°C	Above 55	–	EN ISO 2719
Carbon residue [f] (on 10 % distillation residue)	% (*m/m*)	–	0,30	EN ISO 10370
Ash content	% (*m/m*)	–	0,01	EN ISO 6245
Water content	mg/kg	–	200	EN ISO 12937
Total contamination	mg/kg	–	24	EN 12662 [g]
Copper strip corrosion (3 h at 50 °C)	rating	class 1		EN ISO 2160
Fatty acid methyl ester (FAME) content [h]	**% (*V/V*)**	**-**	**7,0**	**EN 14078**
Oxidation stability	g/m^3	–	25	EN ISO 12205
	h	20	-	EN 15751 [i]
Lubricity, corrected wear scar diameter (wsd 1,4) at 60 °C	μm	–	460	EN ISO 12156-1
Viscosity at 40 °C	mm^2/s	2,00	4,50	EN ISO 3104
Distillation [k, l] % (*V/V*) recovered at 250 °C % (*V/V*) recovered at 350 °C **95 % (*V/V*) recovered at**	 % (*V/V*) % (*V/V*) **°C**	 85 	 < 65 **360**	EN ISO 3405

Figure 22: Standard EN 590 in the European transportation sector for a diesel fuel [21].

3.3.2 Fuel properties

Cetane number

Cetane number characterizes the quality of ignition. In order to find an application in CI engine, fuel needs to have good auto-ignition properties. Insufficient quality of ignition leads to longer ignition delay and as a result poor cold start performance, greater exhaust, noise emissions and high pressure peaks might occur [14]. Increase in cetane number results in lower emissions of CO, HC and NO_x [22]. Reference fuel determines the scale of cetane number: cetane (n-hexadecane) has excellent ignition properties and has number 100, while alfa-methylnaphthalene is characterized by poor ignition and its number is denoted 0. The measurement of cetane number is conducted according to two test procedures. First, EN ISO 5165, is compliant with CFR engine presented in Figure 23. The ignition quality is measured in standardized single cylinder varying compression ratio for constant ignition delay. The Second, EN 15195, is compliant with BASF engine and air/fuel ratio is altered to get a constant and well-defined ignition delay. According to definition a sample of fuel have such a cetane number as a reference fuel with a corresponding concentration of cetane in the mixture. So, if the examined fuel performs the same as a mixture of 60% cetane and 40% alfa-methylnaphthalene, the cetane number is 60. This also applies to fuels with additives.

Figure 23: CFR engine used as a cetane rating unit [23].

Generally, normal paraffins have high cetane number unlike to branched iso-paraffins. Olefins have still high cetane number, but lower than n-paraffins. Naphthenes have medium cetane number and aromatics are characterized by low cetane number. Hydrogenation process in refineries under high temperature and high pressure leads to a rise in cetane number. Especially synthetic diesel can have really high cetane ratings.

Cetane index

A cetane index is a parameter also indicating ignition properties of the fuel. For a need of EN 590 standard, there is an EN ISO 4264 method of calculation based on fuel density and boiling characteristics. Generally, the rise of cetane number is observed with the increase in boiling temperature and drop of density. An increase of boiling temperature results in longer chain components, which ignite easier. An increase of density is followed by the aromatic content growth and it acts adversely to ignition properties [14].

The cetane index is an estimation of the cetane number and is used preferably when the test engine is not available on the spot. The empirical formula called "four-variable equation" was created after approximately 1200 diesel fuels were analyzed. It is an appropriate approximation only for middle distillate fuels from petroleum-derived sources [24]. In addition, it is used rather for blends than for single compounds. It is also not applicable for fuels with additives, which might significantly improve ignition quality. Biodiesel cetane index cannot be assessed on this basis, too.

Fuel property	Recommended range
Cetane number	32.5 – 56.5
Density	805 – 895
10% (V/V) distillation recovery temperature $[^oC]$	171 – 259
50% (V/V) distillation recovery temperature $[^oC]$	212 – 308
90% (V/V) distillation recovery temperature $[^oC]$	251 – 363

Table 4: Recommended range of fuel properties in order to calculate cetane index [24].

Heating value

Fuel energy content can be characterized by the heating value (or in other nomenclature calorific value), which informs about the energy released during combustion. Two types of heating value can be distinguished: higher heating value (or gross calorific value) and lower heating value (net calorific value). In order to measure heating value, fuel is completely combusted and then gases are cooled to the initial conditions, usually STP. The process can be conducted in the specially designed calorific bomb. The difference is based on the state of water molecules in the flue gases – liquid condensates for HHV or vapor phase for LHV. Usually, for ICE purposes LHV is used. This parameter is a measure of energy, which can be theoretically extracted from 1 kg of fuel and indicates (together with density) the necessary amount of fuel delivered by the injection system under specified speed and load of the engine.

Flammability limits

A self-sustained process of fuel burning is observed only in the specific range of volume concentration in the air. For standard conditions STP, lower and upper flammability limits can be distinguished, LFL and UFL respectively. LFL determines the lowest fuel concentration in the air when a spontaneous reaction occurs, for UFL it is the highest possible concentration at which fuel burns. Pressure and temperature are factors influencing those limits and response of the system are gathered in Table 5. While considering combustion other than in the atmospheric air, also oxidizer concentration affects flammability limits.

	$T\uparrow$	$T\downarrow$	$p\downarrow$	$p\uparrow$
LFL	$\downarrow$	$\uparrow$	$\uparrow$	$\approx$
UFL	$\uparrow$	$\downarrow$	$\downarrow$	$\uparrow$

Table 5: Influence of pressure and temperature on the flammability limits [20].

Ignition temperature

A temperature of ignition for the given fuel determines the lowest possible temperature at which generated heat from combustion is higher than losses to the ambient and the process becomes self-sustained [20]. Below that temperature, the self-propagating combustion is not observed unless the external heat is delivered. The ignition temperature and flammability limit can predict the potential for ignition.

Substance	**Molecular Formula**	**Lower Flammability Limit, %**	**Upper Flammability Limit, %**	**Ignition Temperature, $^{\circ}C$**	**References**
Carbon	C	—	—	660	Hartman (1958)
Carbon monoxide	CO	12,50	74	609	Scott et al. (1948)
Hydrogen	H_2	4,00	75	520	Zabetakis (1956)
Methane	CH_4	5,00	15	705	Gas Engineers Handbook (1965)
Ethane	C_2H_6	3,00	12,5	520 to 630	Trinks (1947)
Propane	C_3H_8	2,10	10,1	466	NFPA(1962)
n-Butane	C_4H_{10}	1,86	8,41	405	NFPA(1962)
Ethylene	C_2H_4	2,75	28,6	490	Scott et al. (1948)
Propylene	C_3H_6	2,00	11,1	458	Scott et al. (1948)
Acetylene	C_2H_2	2,50	81	406 to 440	Trinks (1947)
Sulfur	S	—	—	190	Hartman (1958)
Hydrogen sulfide	H_2S	4,30	45,5	292	Scott et al. (1948)

Table 6: Ignition temperatures and flammability limits for common fuels [20].

Volatility

Volatility is a property, which informs about boiling characteristics of the fuel. For a diesel typical temperature range for boiling is approximately $170 - 380^oC$. There is a standardized method EN ISO 345 for measuring the volatility of the mixture. In EN 590 standard, the recovery temperatures are specified:

- at temperature 250^oC less than 65% fraction should be recovered (% on the volume basis),
- at temperature 350^oC at least 85% should be recovered,
- 95% of the mixture should be recovered at a temperature of 360^oC.

Adequate volatility is essential for engine's proper operation. On the one hand, if volatility is too low then power output and fuel economy tend to reduce due to insufficient atomization [14]. On the other hand, if the volatility is too high then also power is reduced because of vapor lock in the fuel system and problems with the nozzle. Lowering the final boiling temperature from 370 to 360^oC was related to the increase of performance and exhaust emission reduction [14].

Density

Density is a physical property, which specifies mass of a certain volume of the fuel in specific conditions. Usually, STP are reference conditions while methods EN ISO 3675 and EN ISO 12185 are used. In EN 590 standard density of standard diesel should be in the range of 820-845 kg/m^3. Density influences spray formation and thus mixing characteristics. Especially it is taken into account when adjusting injection system. Density might be also an indicator of fuel quality. The rising density follows an increase in carbon content of the fuel (caused by the growing length of chain or aromatic content growth). As density rises, the volumetric calorific value of the fuel also increases. Nevertheless, this consideration of density affecting combustion is valid only for petroleum-derived fuels. Synthetic fuels might have higher hydrogen content and thus their gravimetric calorific value is higher.

Viscosity

Viscosity determines the ability of a fluid to resist shear stresses, informs about a possibility of absorbing stresses during deformation. This fluid property is very important for injection system including spraying and atomization. Dynamic and kinematic viscosity can be distinguished. In EN 590 standard, kinematic viscosity of the diesel fuel should be in range $2.00 - 4.50$ and measured by EN ISO 3104 method. It is conveyed in 40^oC and 15 ml of sample is flowing through a capillary tube. Generally, viscosity increases with a drop in temperature. The high viscosity of fuel entails poor atomization and large droplet formation. Moreover, high penetration of the spray jet in the form of a solid stream instead of small droplets influences inadequate air-fuel mixing and results in a worse performance. In addition, for high viscous fluid, fuel spray can hit the cylinder walls during injection and hence cause lubricating oil dilution and eventually lead to higher cylinder material wear. Finally, problems with the delivery system, i.e. fuel pump might be present. On the other hand, low viscosity fuel creates too soft spray not penetrating properly the combustion chamber and affecting poor mixing. In that case, also power loss and rise in specific fuel consumption might be observed. Too low viscosity can induce fuel metering problems due to leakages in the injection pump. Those restrictions determine the operational range of fuel viscosity, which is very important while choosing drop-in fuel.

Flowability at low temperature

Fuel operation at low temperatures is also an important issue. Especially fuel delivery system and injection are affected in a low temperature range. Well igniting paraffins have a shortcoming when it comes to subzero temperature conditions – they tend to crystallize and coagulate. This results in clogging problems. Some kind of solution can be achieved by the proper additives. Indicators of low temperature flowability are as follows:

- Cold filter plugging point indicates the lowest temperature at which fuel is flowable and filtered unimpeded. For fuels without additives, CFPP is just below the cloud point but after adding some flow improvers and anti-settling additives, CFPP can be even 20^oC below the cloud point [14]. CFPP is a better indicator of fuel reliability in low temperatures than cloud point itself because fuel filtering system can cope to some extent with paraffinic crystals. In EN 590 standard there are climate-dependent requirements and they are expressed in different fuel grades. A distinction is made between temperate and arctic winter climates. In Table 7, there are presented fuel grades based on the CFPP value for temperate climates.

Property	Unit	Limits						Test method
		Grade A	Grade B	Grade C	Grade D	Grade E	Grade F	
CFPP	C, max.	5	0	5	10	15	20	EN 116

Table 7: Fuel grades in temperate climates [21].

- Cloud point is a temperature at which paraffin waxes start to crystallize and are getting visible. This temperature depends on the type of the fuel, its origin and refining process. The higher the cloud point, the worse operational suitability of the fuel at low temperatures. In modern diesel cars, this parameter does not play a huge role in contrary to CFPP. In EN 590 there is no specification concerning cloud point.

- Pour point is the lowest temperature at which fuel can be pumped from the fuel tank, hence specifies a theoretical operational limit.

Lubricity

Diesel fuel itself should also act as a lubricant for some parts in the injection system, especially injection pumps and injectors. Unless fuel owns good lubricating properties, then unfavorable wear of such elements can occur. After removing sulfur, fuel does not contain polar substances, which act as wear reducing agents. That is why it is necessary to make a fuel enrichment in the form of adding lubricating additives. EN 590 specifies the maximum allowed wear of element in a test method using high frequency reciprocating rig, which stimulates wear in the injection pump.

Flash point

Flash point is a safety parameter not influencing the combustion process. Some part of a fuel in a closed vessel evaporates while temperature rises. As a consequence mixture of fuel vapor and air forms and finally can ignite when the temperature is high enough and an external source of ignition is delivered. Hence, flash point temperature determines the lowest temperature under normal pressure at which fuel vapors mixed with air in a closed vessel can ignite. For a diesel fuel, the risk of ignition during storage is significantly lower than for gasoline. In EN 590 standard, 55^oC is a minimum flash point temperature, which at the same time limits low boiling compounds in a fuel mixture (initial boiling point for diesel fuel does not need to be specified).

Purity

Proper operation of advanced combustion system in CI engines requires specified restrictions related to the fuel purity. Purity encompasses carbon residue, ash, water and total impurities content. Fuel at the dispensing station should comply with all limits imposed in EN 590 standard for all aforementioned factors in order to avoid problems with pumping, injection and exhaust emissions.

- Carbon residue is measured with EN ISO 10370 test method. The residual 10% fraction of the boiling analysis with the highest boiling temperatures is carbonized. Too high concentration can cause the formation of deposits in injection system and combustion chamber.

- Ash content tells about inorganic compounds in the fuel. It should not be higher than 0.01% on a mass basis.

- Water content describes the total allowable amount of water in the examined fuel and it cannot exceed 200 mg/kg fuel. Especially, in wintertime fuel filter might be clogged by water crystals. The solubility of water in diesel fuel increases with the rise of temperature and aromatics content.

- Total impurities refer to all undissolved materials present in the fuel, i.e. sand particles, rust. Clogging of fuel filter in a case of increased content above 24 mg/kg may occur.

Aromatics

Aromatic HC due to double bonds and cyclic structure are low reactive and hence auto-ignite poorly. Mononuclear aromatics with long side chains exhibit similar properties to normal paraffins. In contrary, polynuclear aromatics significantly deteriorate ignition quality and are assumed to increase pollution formation. In addition, high content of aromatics can also influence operational issues with elastomers and seals. In EN 590 standard, polycyclic aromatic hydrocarbons are restricted to 11% of the mass content. The test method is based on EN ISO 12916 and polyaromatics are measured by means of chromatography and refractivity of the fuel's sample. Results include not only polyaromatic rings content but also side chains, what might be perceived as a drawback of this method.

Sulfur

The content of sulfur is dependent on the fuel, mainly from its origin. It is an undesired element, which has an adverse impact on the engine performance. Higher quantities of sulfur can result in increased SO_2, sulfate and PM formation. In addition, engine oil might undergo acidification process or exhaust aftertreatment system can be destroyed. Due to the acidic property of sulfur, the engine can also experience corrosive wear. Engine oil can partly neutralize acidic content. However, then it requires more frequent change intervals. All above considerations indicate that desulfurization of fuel is crucial process prior combustion. In the EU diesel fuel should be "sulfur-free", meaning that it is allowed 10 mg per 1 kg of fuel [14]. The measurement standards shall be compliant with standard EN ISO 20846 and EN ISO 20884.

The engine tolerance of the sulfur depends upon the type of an engine. Low-speed engines can tolerate more sulfur as they tend to operate with steady temperature and low fluctuations. Also, higher output and operating temperature lessen the influence of sulfur contained in the fuel [25].

Corrosiveness on metals

The contact of a fuel with metal supply lines and elements can lead to corrosion, adverse rust formation and final destruction. Corrosiveness of a fuel is influenced by factors such as moisture, oxygenates and sulfur compounds. In order to protect metal elements, special additives are added. Especially corrosion of copper materials, including pump elements, not only affects the damage of component but also results in the formation of molecular impurities as a copper is a very reactive metal [14]. In standard EN 590 there is a limitation for corrosiveness of the fuel and copper strip corrosion should have rating 1. The test method based on ISO EN 2160 requires immersing copper strip in the diesel fuel for 3 hours at 50^oC and corrosion behavior is estimated. A complementary method is a measuring of acidity of fuel in order to determine tendency for corrosion.

Stability

Stability is an important property, which affects the storage and expiration date of fuel. It determines the resistance of the fuel to undergo chemical changes in the contact with the environment. Oxidation stability refers to oxidation process and later polymerization of fuel when it is stored for extended period of time. This inevitable process might lead to the clogging of the fuel filter. Oxidation in principle is an attachment of oxygen, usually to unsaturated olefins. The rate of oxidation is influenced by such factors as temperature, oxygen availability, the presence of catalytic species, light delivered to the system [25]. Additives called antioxidants can strongly inhibit the formation of free radicals and in consequence, prevent further oxidation and polymerization.

Standard EN 590 determines an oxidation stability by an EN ISO 12205 technique while it is measured in open vessel artificially aerated with pure oxygen for 16 hours. The limit of formed resinous compounds should not exceed 25 g/m^3. An alternative way of measurement for diesel fuels, which contain FAME, is conducted based on EN ISO 15751. In that case, air is passing fuel sample and then the fuel-vapor mixture is fed to distilled water while conductivity is measured until a steep growth is observed. In EN 590 the minimum time up to reaching this rise is set to be 20 hours.

Property	Unit	Fuel		
		Neste Pro Diesel 2017	**Neste Futura Diesel 2017**	**ST1 Diesel Plus 2017**
Cetane number	-	60	54	63
Cetane index	-	55	55	63
Density at 15^oC	kg/m^3	826	825	805
PAH content	$\%m/m$	1	2	1
Sulfur content	mg/kg	3	5	5
Flash point	^oC	74	63	65
Carbon residue	$\%m/m$	< 0,01	<0,02	< 0,02
Ash content	$\%m/m$	< 0,001	< 0,001	< 0,001
Water content	mg/kg	40	53	70
Total contamination	mg/kg	2	3	4
Copper strip corrosion	class	1a	1	1
FAME content	$\%V/V$	0	0	1,5
Oxidation stability	g/m^3	3	2	2
Lubricity	μm	380	300	350
Viscosity at 40^oC	mm^2/s	3	3	3,1
Distillation at 250^oC	$\%V/V$	24	32	25
Distillation at 350^oC	$\%V/V$	97	94	95
Distillation temperature of 95% fraction	^oC	338	351	351
Cloud point	^oC	-14	-5	-12
CFPP	^oC	-26	-15	-22

Table 8: Typical commercial Finnish diesel fuel property values measured in compliance with European norm EN 590. Based on [26], [27], [28].

3.3.3 Fuel additives

Fuel additives, usually in trace amounts, are used in order to improve the fuel quality. Lubricity improvers enhance the lubrication properties whereas cetane number enhancers have a positive effect on the autoignition quality. Fuel additives are added to a fuel in a refinement process by fuel producers. Many types of additives are used currently in the market and an approach to classify them with respect to their function is shown in Figure 24.

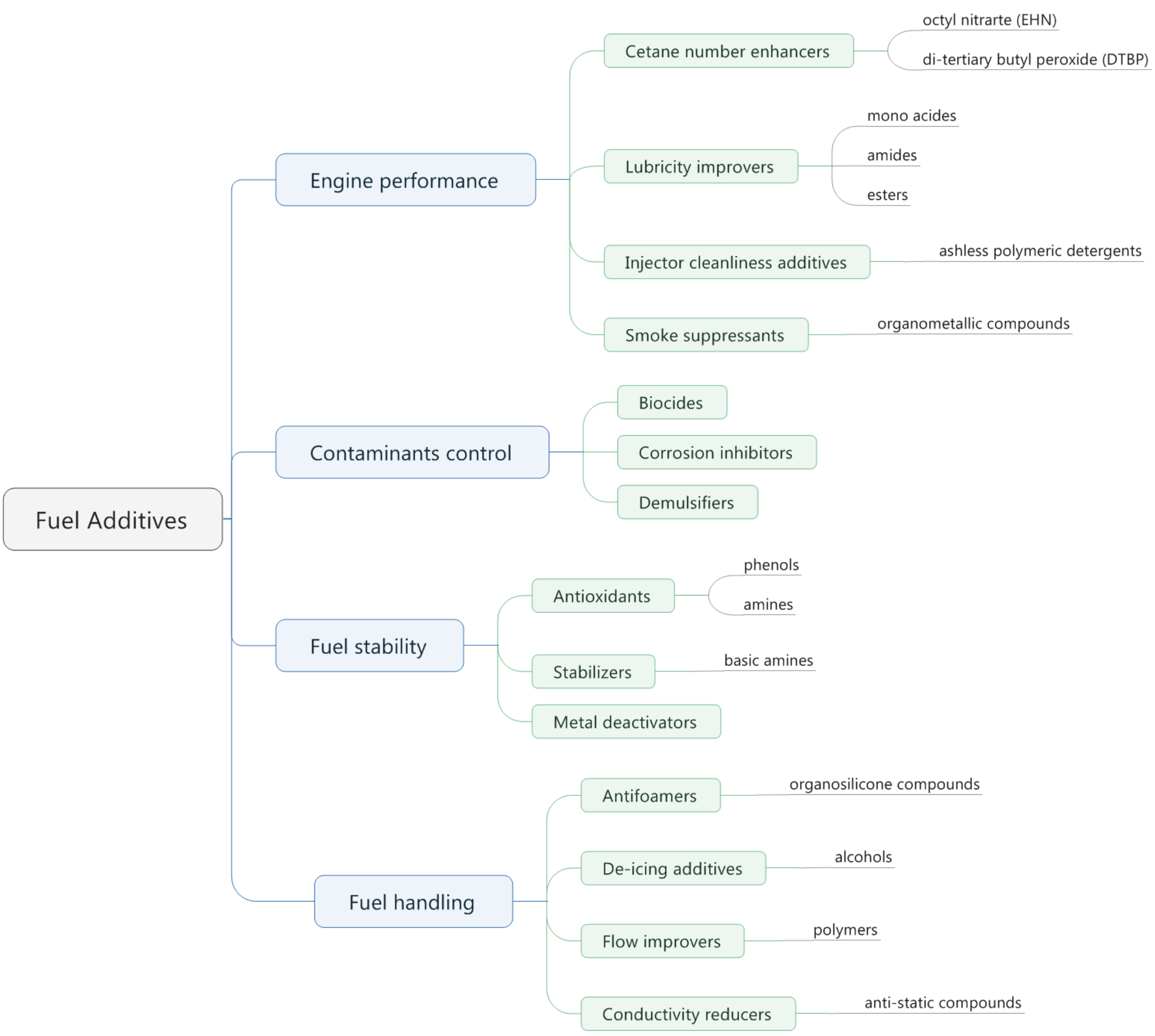


Figure 24: Classification of diesel fuel additives (based on [22]).

3.4 Emission control systems

Emissions from modern engines are reduced due to progress in engine combustion technology and also in aftertreatment systems deployed in the vehicles. Improvement in tailpipe emissions results from more and more stringent requirements dictated by European law. Therefore, manufacturers need to gradually improve current systems and develop new technologies. Significant reductions can be observed when comparing new and old diesel engines. The design of combustion system is a crucial factor, which in previous years enabled significantly lower emissions.
Although significant reductions in emissions have been achieved through the combustion system design in recent years, there is still need for more advanced aftertreatment technologies in order to comply with the European requirements. Oxidation catalytic converters, particulate filters, EGR, SCR, NO_x storage catalyst and Miller timing are in use in common modern diesel engines.

3.4.1 In-engine modifications

Injection system's recent modifications brought significant emission reductions. Firstly, very high injection pressure enhances fuel atomization and smaller droplet formation, which is followed by easier vaporization of fuel and eventually more homogeneous mixture and shorter ignition delay. Secondly, utilization of very precisely shaped, multihole nozzles enabled better penetration of combustion chamber. Thirdly, a very accurate timing of injection is possible by the fast responding piezoelectric injectors. That is why in current injection system special timing patterns can be used including pre-, main and secondary injection. All above improvements led not only to better emission characteristics but also tremendously increased fuel economy.
Increased air swirl enabled better fuel-air mixing.
The cooling system in turbocharged cars entailed lower final temperature and this was followed by decreased NO_x emissions.
Lowered oil consumption was achieved by better sealing and limiting the seepage of crankcase lubricating oil through the piston rings to the combustion chamber [22].

Exhaust gas recirculation (EGR)

Exhaust gas recirculation is a unit responsible for lowering NO_x emissions. It directs part of exhaust gases again into the combustion chamber. Recirculation rate can reach up to 50% and it depends on the speed and load of an engine [11]. Gases are collected before the turbocharger and cooled in the heat exchange unit and then put in the intake manifold. The working principle is based on the decreasing of final temperature during combustion. Exhaust gas can be treated as an inert gas, which does not take part in a combustion process. However, some heat is used for raising its temperature. This results in decreased NO_x formation as a consequence of lower final temperature. The recirculation rate is controlled by built-in engine control unit. Usage of EGR is also followed by some small power loss of the engine. The EGR unit is presented in Figure 25.

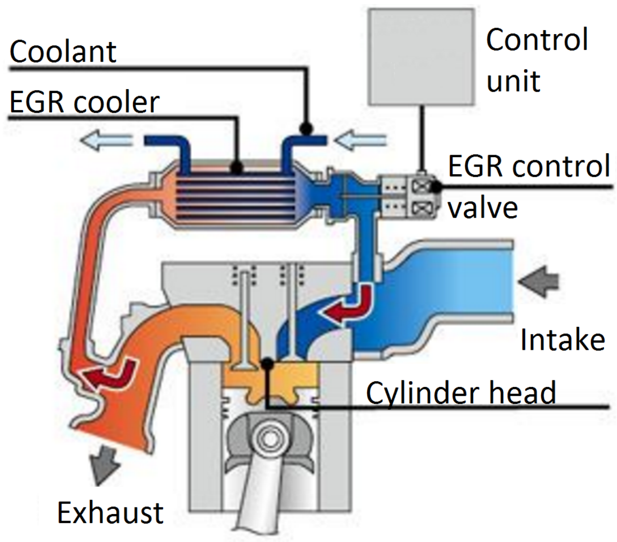


Figure 25: Schematic of EGR [29].

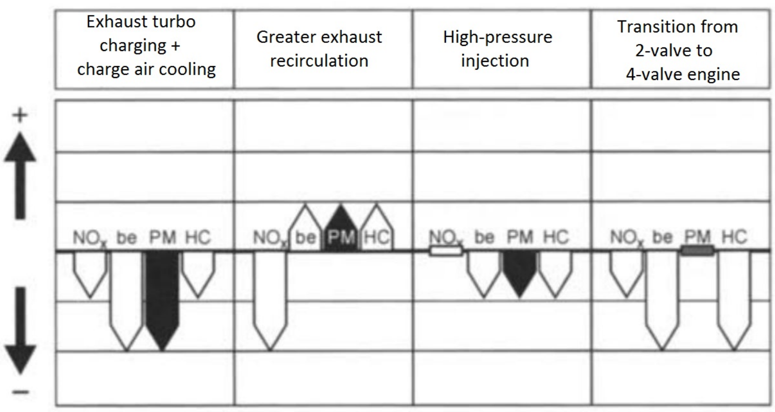


Figure 26: Combustion system designs impact on the emissions; notation: + rise, − drop in emissions [11].

Miller timing

Miller timing is another technology used in order to decrease NO_x emissions. Miller timing refers to Miller process, in which effective compression stroke is shorter than expansion stroke. Such an action is attainable by proper shifting the inlet valve closing time. Inlet valve can be either early or late closed in reference to the BDC position of the piston. Taking into account ideal process, thermal efficiency should be slightly lower than for conventional diesel cycle. However, lower temperature results in lower heat losses and actually thermal efficiency tends to be higher than in standard valve timing. In order to implement Miller timing, turbocharging is a necessary action. Single or two stage turbochargers (Figure 19) might be applied. Consequently, the final combustion temperature is reduced for a constant engine output - this leads to decrease in NO_x emissions [30] and additionally lowers fuel consumption.

3.4.2 Aftertreatment systems

Oxidizing catalytic converters (DOC)

Diesel oxidizing catalytic converter consists of three main components shown in Figure 27: honeycomb made of ceramic or metal used as a substrate, porous coating of Al_2O_3 and precious metal being a catalytic center where oxidation reactions take place [11]. DOC operates at high temperature and removes unburned HC and CO converting them into CO_2 and H_2O. It acts continuously and does not need regeneration unless its surface is deactivated, i.e. by sulfur. Due to a higher concentration of PM and lower exhaust temperature (up to 800 ^oC), the efficiency of DOC is lower than TWC in a case of SI engine. However, modern diesel combustion systems emit very small amounts of unburned HC and CO.

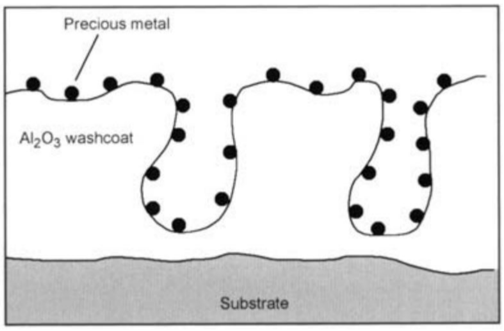


Figure 27: Surface of oxidizing catalytic converter [11].

Diesel particulate filter (DPF)

For the street traffic purposes, PM is considered as any mass that can be filtered and weighed by the gravimetric method at 325 K. For the environmental purposes, two types of fine PM are distinguished: $PM10$ and $PM2.5$ with particles of diameter below 10 μ and 2.5 μ respectively. Diesel particulate filter traps the PM from the exhaust gases. Soot particles are accumulated, however capacity of DPF is limited. This requires soot disposal and regular burn-off. DPF is regenerated actively after certain loading capacity had been reached, usually 70% and it means regeneration every 300-2000 km [14]. The catalytic coating improves regeneration process, which is conducted under elevated temperature conditions obtained by i.e. usage of throttling plates for the intake air. Then retarded post injection is applied and some of the unburned fuel initiate combustion inside the DPF filter. In practice, the regeneration process is led on the highway during a stable operation lasting at least 10 minutes or in the control station. The clogged DPF can cause loss of power and a higher thermal load of the engine. Modern particulate filters are ceramic wall flow filters and their honeycomb material might be: cordierite, silicon carbide, aluminum titanate. In the market there are also SCR-catalyzed DPF, employing simultaneous NO_x reduction [31].

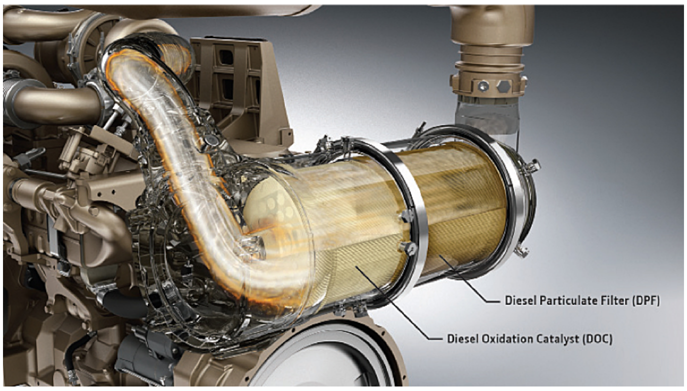


Figure 28: DPF and DOC as one unit in diesel aftertreatment system [32].

Selective catalytic reduction (SCR)

A selective catalytic reduction is a current technology, mainly used for heavy-duty engines in trucks and non-road vehicles. SCR is another method for reducing NO_x emissions. SCR systems utilize urea solution held in a separate tank, which is injected into the exhaust system before the selective catalyst. Urea solution forms eventually ammonia, which reacts with NO_x over the catalyst and nitrogen oxides are reduced to the molecular nitrogen. Significant NO_x emission reductions, up to 90% might be achieved, as well as a decrease in HC and PM concentration. In Europe, commercially available AdBlue is used in heavy-duty diesel trucks in order to comply with Euro regulations. It is a corrosive solution and thus it requires special distribution systems and should be refilled periodically in the dispensing station. In order to avoid ammonia leakage into the atmosphere, ammonia slip catalyst is mandatorily required after SCR system.

NO_x storage catalyst

NO_x storage catalyst is a technology for reducing mainly NO_x and additionally unburned HC and CO emissions. The operation of this catalyst involves deposition of NO_x on the surface area. This process requires lean conditions. In the beginning, nitric oxides (NO) are oxidized on a precious metal to nitrogen dioxides (NO_2) and then they are bonded to the catalyst structure, for example barium carbonate structure. Hence, the storage material is consumed during an operation and requires periodical regeneration in order to maintain high efficiency. Rich conditions are appropriate for regeneration of catalyst while CO and unburned HC cause a nitrogen to be released in a form of NO from the accumulated structure. Further on, nitric oxides are reduced to N_2 on the precious metals of the catalyst surface. The temperature for regeneration might be even below 100 ^oC [31]. NO_x storage catalyst can be poisoned by the sulfur and then much higher temperature for regeneration must be attained.

4 Methodology

4.1 Problem approach

Meeting an objective of ADVANCEFUEL project is an extremely challenging task. It is very important in the very beginning to carefully draw the structure of the problem and understand correctly goals. Clear deliverables should be provided as final results from the thesis work. The outcome is satisfactory when the models can properly predict the impact of fuel properties on engine performance. Planned actions towards final result include three main subsections presented in Figure 29. First one relates only to fuels. It encompasses identification of most prominent alternative fuels, recognition of the most relevant properties and estimation of fuel blend final properties. The second subsection is related to the engine. Such indicators as fuel consumption, efficiency and influence on components are analyzed. An exhaust system is the third subsection and mostly concentrated on GHG emissions and aftertreatment technologies. The simultaneous analysis of fuel and engines leads to co-optimization process. There is also one big project in the United States called Co-Optima analyzing chemical compounds and their potential for ICE application [33]. It has already some interesting results for SI engines but CI engines are still under initial phase of research.

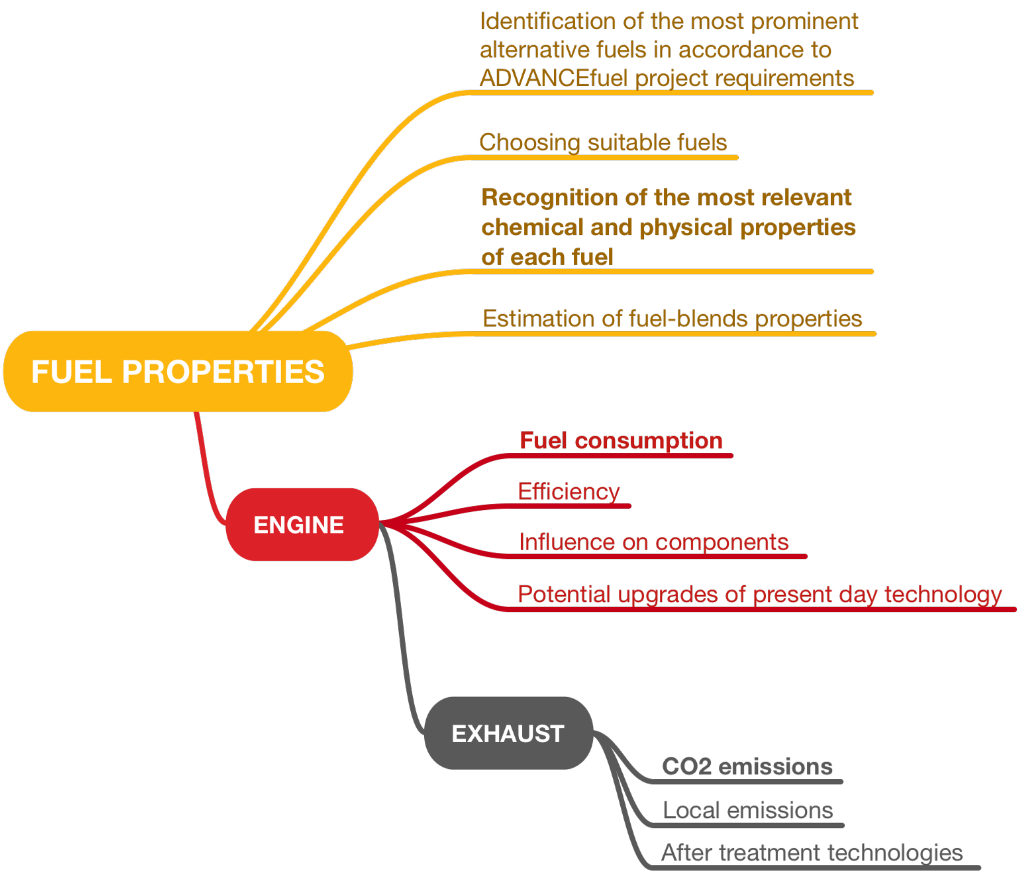


Figure 29: Schematic presentation of problem structure.

In principle, the model should take into account fuel and its properties. On the other hand, type of engine (light-duty, heavy-duty, marine or aviation) and operational conditions should be considered at the same time. From the engine side, there are parameters, which characterize combustion and the most important among them are: ignition delay, maximum heat release rate, cylinder pressure. However, they are not contained in this thesis. The main aim of the model is not a physical description of alternative fuels behavior and detailed explanation of combustion characteristics. Instead of that, the model should predict the final impact on engine performance, which can be observed by the end-user. The assessment of the fuel properties impact on engine performance is done via such indicators as fuel consumption and emissions. In summary, the final model needs to connect the fuel properties with engine operation and the outcome should take into account both of them. In the ideal case, the results should enable decision makers or fuel producers to estimate engine performance indicators based only on the known set of fuel properties. A schematic approach to the task is presented in Figure 30.

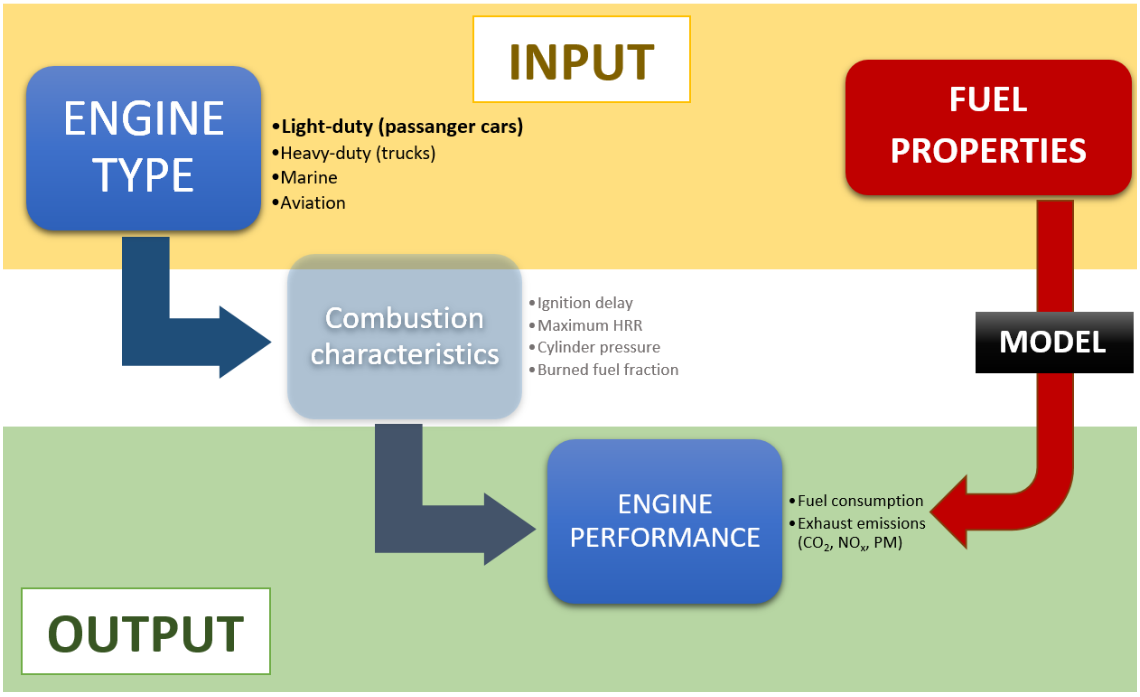


Figure 30: A final approach to the designated task in order to meet an objective of ADVANCEFUEL project.

4.2 Selection of fuels

For the purpose of this work, there are few fuels taken into account. Among the most important are fossil-based diesel, FAME, HVO, BTL/GTL. All fuels are tested as drop-in fuels where no in-engine modifications are required. However, for example FAME is not fully compatible with modern DI diesel engines when using higher concentration in blends with standard diesel. That is why for some fuels the blending-wall is determined. Short characteristic of each fuel is presented below. More detailed specification of CI engine fuels is attached in Appendix A. Beside analyzed fuels, also straight vegetable oil (SVO) and dimethyl ether (DME) can be utilized in CI engines. However, those are not drop-in fuels. Moreover, ethanol is another fuel for CI engine purposes but it needs significant portion of additives. Properties of DME, SVO and pure ethanol are also presented in Appendix A.

Standard diesel

Standard diesel is a fossil-based fuel used in CI engines. It is a fraction of crude oil heavier than gasoline, produced in refinery during refinement of oil. In the European market, diesel fuel should comply with norms specified in EN 590. Despite the fact that this standard determines allowed range of various properties, there might be significant differences when comparing diesel fuels from separate distribution lines. The final properties of diesel depend on the origin of crude oil, refinement process and blending practices. It is important to remark that there is no universal or reference diesel fuel. The final values should be only within the ranges given by standards, which in some cases are quite wide, i.e. according to EN 590 density should be higher than 820 but lower than 845 kg/m^3.

FAME

FAME diesel is a traditional biodiesel, which consists of fatty acid methyl esters. It is the first generation biofuel produced by transesterification process from edible oils such as rapeseed, sunflower or palm. The advantages over diesel are better lubricity, reduced toxicity of emissions [34]. On the other hand, high viscosity, worse stability and low temperature characteristics make the biodiesel less attractive than HVO. Rather limited potential in the future is anticipated due to competition with food crops. FAME fuels have their own specification - EN 14214. The main differences in this standard are related to higher density and viscosity of biodiesel. The limits are 860-900 kg/m^3 and 3,5-5,0 mm^2/s for density and viscosity, respectively. In addition, ester content characteristic for FAME is included in that norm. The oxygen content is another significant difference when compared with standard diesel, pure biodiesel can have around 10% of oxygen content (mass based percentage) [35]. FAME can be used as standard diesel blending component but in EU the limit is 7% (volume based percentage).

HVO

HVO abbreviation denotes hydrotreated vegetable oil and it refers to paraffinic diesel fuel. HVO is produced from vegetable or animal oils in the process of hydrotreating catalysis. This fuel is classified as high cetane number paraffinic diesel. The advantages of HVO are good ignition characteristics, mainly paraffinic HC composition. In addition, a good potential of that fuel is caused by the fact that it can be produced from waste cooking oils. Moreover, a final end-use characteristic is reported to be better than for standard diesel and when some modifications are applied, the gains may be even more significant [36]. The HVO fuel should comply with separate standards for paraffinic fuels - EN 15940. It is mainly due to the lower density of this fuel, in standard the range is 765-800 kg/m^3. Also, the cetane number should be above 70.

BTL and GTL

BTL is biomass-to-liquid diesel classified as high cetane number paraffinic diesel. It can be produced directly from the cellulosic feedstock by Fischer-Tropsch synthesis and can be counted as second generation biofuel. Final physical and chemical properties are close to HVO due to the similar chemical composition of those fuels - mainly a mixture of straight chain and branched paraffinic hydrocarbons. Similar performance of BTL and HVO should be expected. GTL is gas-to-liquid fuel and might be either fossil-based or produced from renewable sources. It indicates also similar properties as BTL. EN 15940 is a standard for all paraffinic fuels including BTL, GTL and HVO.

Drop-in fuels

Drop-in fuel definition refers to fuel, which can be directly used in current engines without any modifications. There are no negative implications or adverse effects observed while using such a fuel in CI engine initially designed for a standard diesel. *Blending-wall* is a maximum limit for a specific component in a blend, usually expressed in volume percentage. This definition is related closely to drop-in fuels. Below the blending-wall, fuel blend is considered as a drop-in fuel. According to European fuel standards, for ethanol blending-wall is 10% due to EN 228 and for FAME biodiesel it is 7% due to EN 590.

4.3 Fuel properties identification and classification

As described in section 3.3 of the thesis, there are many fuel properties, both physical and chemical, which influence usability of the fuel. For the purpose of this thesis, the most important properties were categorized in several usability groups. The main categories with respect to effect on engine performance are presented in Figure 31. The groups distinguished are as follows: the amount of fuel handled by injection system, ignition characteristic, mixing and combustion, supply system, exhaust emissions, safety and storage. In the first category, lower heating value and density are the main properties. The ignition characteristic is determined by cetane number, autoignition temperature and flammability limits. In the process of mixing and combustion the key role play volatility, viscosity, density and oxygen content. Supply system and operational issues are mostly influenced by viscosity, lubricity, density and low temperature flowability. Exhaust emissions depend on the content of aromatics, sulfur, total contamination and also oxygen. Safety and storage are determined by flash point, corrosiveness on metal, oxidation stability and compatibility with components' materials.

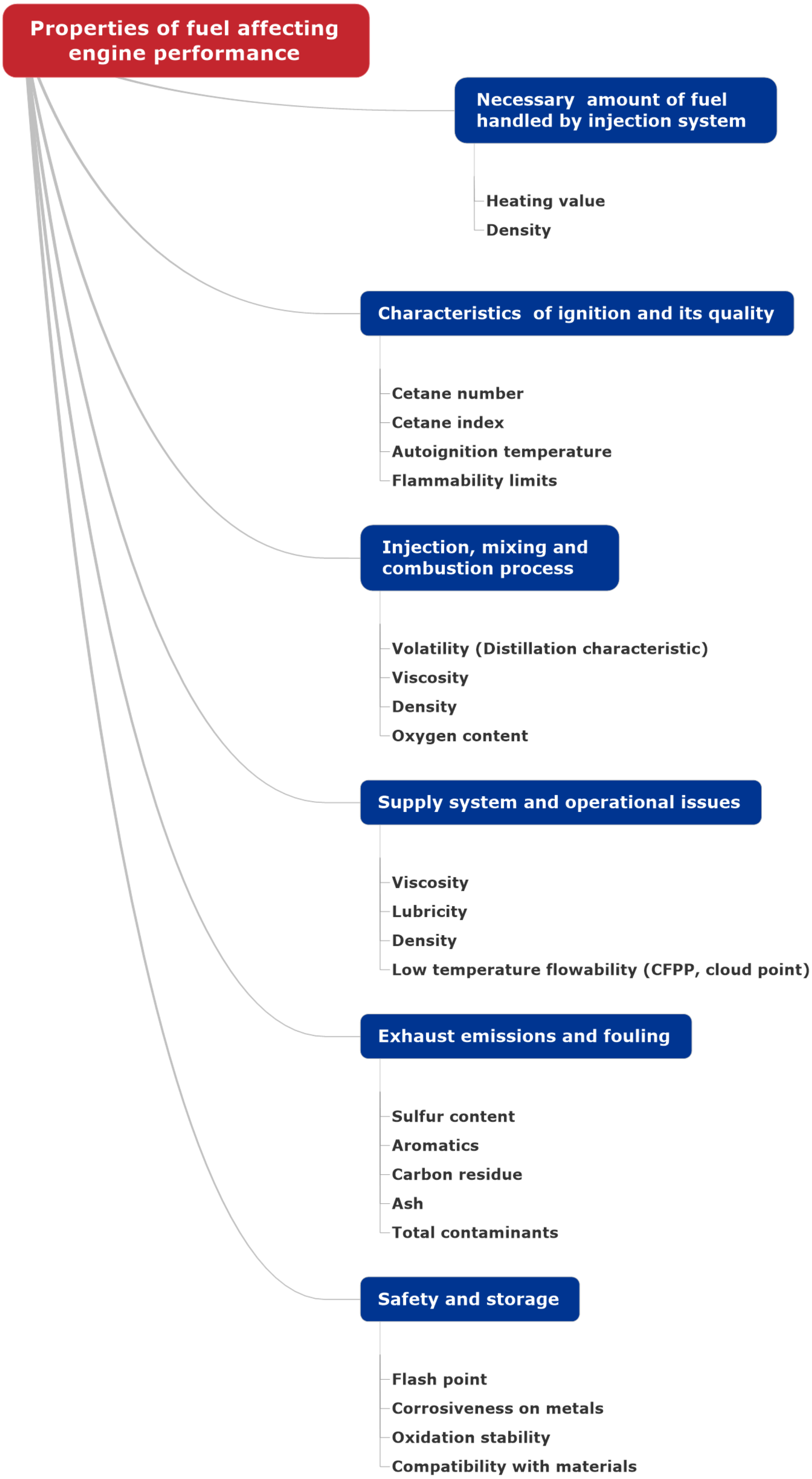


Figure 31: Classification of fuel properties regarding the impact on engine performance.

Created graph (Figure 31) was used in further studies in order to select the final properties for modeling purposes. First three groups affect fuel consumption the most. It was decided to select lower heating value as a representative from the first group reflecting the amount of fuel handled by injection system. From the second category, cetane number was chosen as the main parameter for ignition quality. Density, viscosity and oxygen content from the third group were identified to be the most influential on injection, mixing and combustion process.

Other types of fuel property classification are presented in Figure 32 based on [22]. The first one indicates that bulk and minor type properties can be distinguished. The bulk type property is determined by the overall composition of the fuel treated as one substance, i.e. density, viscosity and lower heating value. In contrary, the minor type property is determined by specific minor component, here lubricity, flash point or sulfur might be mentioned. The second classification takes into account period of the effect caused by separate property. The impact of some properties can be observed immediately, like in a case of cetane number, volatility, density, heating value. Meanwhile, for other properties, the time frame of effect is moderate and it is in case of sulfur content, lubricity, flash point or stability.

All selected for modeling properties are bulk type properties with the immediate time frame of effect, except oxygen content, which has a moderate time of effect on final performance. It is also good to mention that cetane number can be improved slightly by means of fuel additives. Where applicable, fuel and fuel blend property values were taken directly from the source presenting engine performance. When it was not possible, the data were extracted from other sources and linear regression was applied in order to obtain values for specified blend properties.

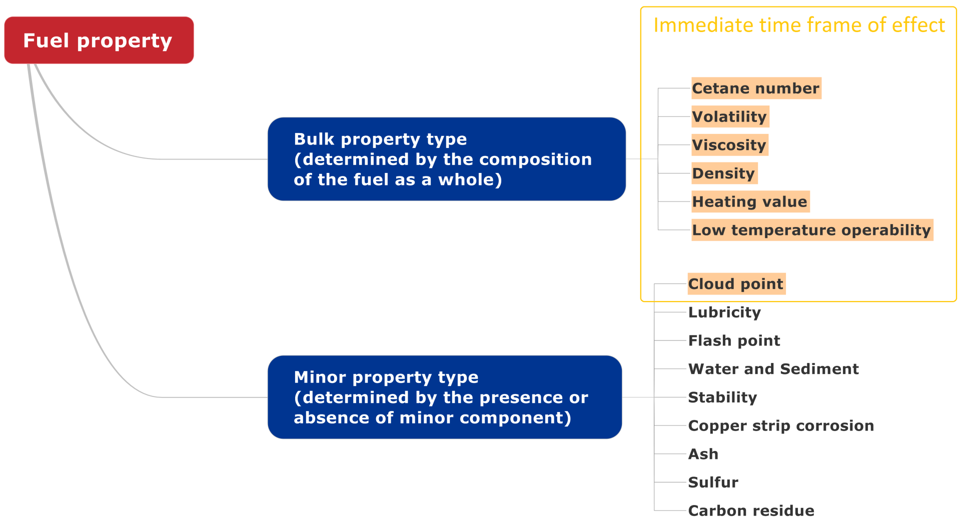


Figure 32: Two types of the division for fuel properties: bulk vs minor properties and immediate vs moderate time frame of effect properties (based on [22]).

4.4 Steady state approach

While examining fuel and fuel property impact on engine performance, the operating conditions should be specified. The most convenient way to make measurements on alternative fuels is to apply steady state conditions. This results in specified engine speed (speed in rpm) and load (torque in Nm). Alternatively, engine speed can be expressed by mean piston speed and torque replaced by brake mean effective pressure. Such fixed conditions represent single point from engine operational map. In the majority of articles and publications, the experiments were conducted just for few steady state conditions. A great part of available results was based on adjusted experimental set-ups, which not always reflect the reality in a good way. The implications of using such a data could bring outcomes not consistent with actual performance, especially with real driving conditions. When a modern car is tested on a chassis dynamometer then obtained results are much more reliable. During very extensive review done for the purpose of this thesis, mostly publicly available sources were used. Articles about alternative fuels, which included both exact fuel property specification and impact on engine performance, were taken into account in priority. Many articles were examined, afterwards, initial data were extracted and compared. The analysis was divided into two steps.

The first step included a selection of articles with only one single fuel - RME biodiesel. The moderate conditions of operation were chosen for each engine. The aim was to examine how the fuel consumption shifts when changing the blend ratio of biodiesel and standard diesel in different engines. Four most promising researches with different engines were selected, each shortly described below.

Fuel properties of RME biodiesel					
RME blend %	**LHV [MJ/kg]**	**Density at 15 C [kg/m3]**	**Viscosity at 40 C [mm2/s]**	**CN -**	**Oxygen content %m**
0	42,5	853,4	3,50	51,6	0,0
10	41,9	857,0	3,90	51,9	1,1
20	41,4	859,0	4,08	52,1	2,2
50	40,1	865,1	4,47	52,9	5,5
100	38,3	879,4	5,48	54,2	10,9

Table 9: Fuel properties of RME biodiesel blends.

- Source A: Tesfa, B., *Investigations into the Performance and Emission Characteristics of a Biodiesel Fuelled CI Engine under Steady and Transient Operating Conditions.*, 2011. [37]
  It is a doctoral dissertation from University of Huddersfield, Great Britain. The main aim was an examination of traditional biodiesels with three different types of feedstock: rapeseed, corn and waste oil. For measurements 4.4 liter, four-cylinder, direct injection turbocharged diesel engine JCB brand was used. The maximum power of the engine was reported 74.2 kW and maximum torque 425 Nm at 1300 rpm, the compression ratio of 18.3:1 and bore-to-stroke

ratio 103/132 *mm*. Visible differences were observed when comparing all the biodiesel fuels with standard diesel. Only slight variations could be noticed when comparing biodiesels between themselves due to similar property specifications. The LHV, density and viscosity values were taken directly from that source [37], oxygen content from [38] and cetane number from [39]. The values of fuel blend properties are collected in Table 9. Blends of RME tested during research: 0%, 10%, 20%, 50%, 100%. Engine operational condition selected for analysis are as follows: 105 *Nm* and 1900 *rpm*.

- Source B: Elsanusi, O.A., et al., *Experimental investigation on a diesel engine fueled by diesel-biodiesel blends and their emulsions at various engine operating conditions*, 2017. [40]
  It is a journal paper from Applied Energy. The Canadian research examined the impact of canola biodiesel on engine performance - canola characteristic is very close to rapeseed biodiesel. The measurements were conducted on HATZ 2G40 engine, which is two-cylinder direct injection diesel engine with the displacement of 1.0 liter, bore-to-stroke ratio of 92/75 *mm*, compression ratio 20.5:1 and power 17 kW. Examined fuel blends: 0%, 10%, 20%, 30%, 40%. Conditions chosen for comparison with other sources: medium load and 2100 *rpm*.

- Source C: Tsolakis, A., et al. *Engine performance and emissions of a diesel engine operating on diesel-RME (rapeseed methyl ester) blends with EGR (exhaust gas recirculation)*, 2007. [41]
  The measurements in Great Britain were run on one-cylinder 0.7 liter naturally aspirated direct injection diesel engine featured with 15.5:1 compression ratio, 98/102 *mm* bore-to-stroke ratio and 8.6 kW power. RME biodiesel was tested at two conditions, for analysis following conditions were taken into account: speed of 1500 *rpm* and load 20 Nm what corresponds to 4.5 *bar* of IMEP. Following fuel blends were considered: 0%, 20%, 50%, 100%.

- Source D: Labeckas, G., Slavinskas, S., *The effect of rapeseed oil methyl ester on direct injection diesel engine performance and exhaust emissions.*, 2006. [42]
  Paper from Energy Conversion and Management includes research from Lithuania. RME biodiesel blends were tested on four-cylinder, 4.75 liter, naturally aspirated diesel engine with compression ratio 16:1, bore-to-stroke ratio 110/125 *mm* and 59 kW power. Standard diesel and RME blends were tested at three operating conditions. Moderate conditions with load characterized by IMEP equal 5 *bar* and speed 2200 *rpm* considered during analysis. Data were available for given blends: 0%, 5%, 10%, 20%, 35%, 100%.

The second step included a comparison of completely different fuels using the same engine. It was crucial to select the most reliable source with modern technologies. Results from IEA AMF project called "*Synthesis, Characterization and Use of Hydro-Treated Oils and Fats for Engine Operation*" were used [43]. Thanks to the kindness of the Author, Benjamin Stengel from Rostock University in Germany, it was possible to present the impact of totally different fuels on one modern and representative engine. In that part HVO, FAME and enzymatic FAME were compared in terms of engine operational maps. Enzymatic FAME, in that case, refers to RME biodiesel produced by enzymatic reactions instead of transesterification process. Fuel exact specification is listed in Table 10 together with EN 590 and EN 14214 standard limits. Pure alternative fuels were tested in a wide range of engine operational conditions and then compared to standard diesel. The measurements were performed on modern EURO VI passenger diesel engine from Volkswagen Passat. This engine represents the current market engine with advanced aftertreatment system deploying DOC, DPF and SCR. Detailed engine specification is given in Figure 33.

Property	Test name	Units	EN 590		Tested fuels			EN 14214	
			Min	Max	Standard diesel	HVO (NExBTL)	E-FAME (RME)	Min	Max
Lower Heating Value	bomb calorimetry	MJ/kg			42,517	43,846	37,309		
Cetane Number	ASTM D613		51		53,1	74,7	51,9	51	
Calculated Cetane Index	ASTM D4737		46		50,2	78,3			
Density @ 15 C	ASTM D4052	kg/m3	820	845	838,8	778,8	882,3	860	900
Kinematic Viscosity @ 40 C	ASTM D445	mm2/s (cSt)	2	4,5	2,714	2,868	4,245	3,5	5
Corrected Flash Point	ASTM D93	C	>55,0		63,5	78	141	101	
Cloud Point	ASTM D5773	C	Report	Report	-6,1	-32,1	-0,5	Report	Report
CFPP	ASTM D6371	C	Report	Report	-27	-42	-4	Report	Report
Oxidation Stability @ 110 C	EN 15751	hours	20		12,3		2,4	8	
Copper Corrosion	ASTM D130		Class 1	Class 1	1a	1a	1a	Class 1	Class 1
Wear Scar Diameter	ASTM D7688	um		460	220	400			
Distillation 95% Recovered	ASTM D86	C		360	347,4	293,6			
% Recovered at 250C	ASTM D86	volume %		<65	37	8			
% Recovered at 350C	ASTM D86	volume %	85		96	>97			
Distillation IBP	ASTM D86	C			168,5	190			
Distillation 50% Recovered	ASTM D86	C			270,4	277,7			
Distillation FBP	ASTM D86	C			357,7	301,8			
Distillation Residue	ASTM D86	volume %			1,4	1,3			
Total Sulfur	ASTM D5453	mg/kg		10	7,6	<1	2,5		10
Water Content	ASTM D6304	mg/kg		200	55	20	158		500
Biodiesel Content	ASTM D7371	volume %		7	6,35	<1,00			
Carbon Residue, 10% Bottoms	ASTM D4530	mass %		0,3	0,01	0,01			
Ash Content	ASTM D482	mass %		0,01	0,005	0,003			<0,005
Particulate Contamination	ASTM D5452	mg/L		24 (mg/kg)	0,84	10,45	10,5		24 (mg/kg)
Total Insolubles	ASTM D2274	g/m3		25	1,1	1,1			
Manganese (Mn)	ASTM D7111	mg/kg		2 (mg/L)	<0,01	<0,01			
Free Glycerin	ASTM D6584	mass %					<0,001		0,2
Total Glycerin	ASTM D6584	mass %					0,015		0,25
Total Monoglyceride	ASTM D6584	mass %					0,012		0,7
Total Diglyceride	ASTM D6584	mass %					<0,09		0,2
Total Triglyceride	ASTM D6584	mass %					0,001		0,2
Acid Number	ASTM D664	mg KOH/g					0,83		0,5
Ester Content	EN 14103	mass %					95,3	96,5	
Linolenic Acid Methyl Ester Content	EN 14103	mass %					1,9		12
Polyunsaturated Methyl Ester	EN 14103	mass %					<0,1		1
Methanol Content	EN 14110	mass %					0,04		0,2
Iodine Value	EN 14111	g of I/100g					116		120
Na and K, combined	EN 14538	ppm (m/m)					<1,0		5
Ca and Mg, combined	EN 14538	ppm (m/m)					<1,0		5
Phosphorus Content	EN 14538	ppm (m/m)					<2,0		4

Table 10: Measured values of fuel properties for diesel, HVO, E-FAME and limits for standards EN 590 and EN 14214. Based on data from IEA AMF report [43].

Test engine	VW Passat CBAC
Displacement	2.0 liter / 1,968 cm^3
Engine type	4 – cylinder, 16 valves
Rated output	103 kW at 4,200 min^{-1}
Max. torque	320 Nm at 1,750 – 2,500 min^{-1}
Stroke	95.5 mm
Bore	81.0 mm
Injection	Common-Rail-Injection (second generation)
Exhaust after treatment	DOC – DPF – SCR
EGR	Cooled high-pressure EGR
Turbocharger	Turbocharger with VTG

Figure 33: Specification of modern diesel engine complying with EURO VI norms used in passenger car [43].

4.5 Test cycle procedures

The task of the ADVANCEFUEL project required creating a universal model, which could be applied to new fuel blends. The main interest was to predict the engine performance for real driving conditions and to show effects from the end-user point of view. During regular usage of the engine in everyday life, many steady states' effects contribute to the overall performance. Moreover, there are also transient conditions, which cannot be approximated by steady state measurements. Considering those facts, it was concluded that steady state approach could bring not representative outcomes. In addition, there is a lot of contradiction in literature, some results are not in line with others. In reviews about biodiesel, there are collected recent researches and compared with each other. It turns out that in some experiments thermal efficiency grows while increasing blending ratio but the opposite effect is observed in other measurements [44]. Of course, it can be partly justified by different set-ups and various engine specification, which has also very significant impact on the final result. All mentioned above statements made a steady state analysis inappropriate and nonfeasible approach to obtain a general model.

The new alternative technique was needed and driving cycle test procedures were proposed. New European Driving Cycle (NEDC) and Worldwide Harmonized Light Vehicles Test Cycle (WLTC) are the main test procedures in the European market. Those methods are established by legislation and new vehicles are tested accordingly. Moreover, the results from test procedures should comply with EURO norms concerning emission levels. NEDC is older test procedure, which is currently being replaced by the WLTC. The advantage of driving cycles over steady state measurements is fact that they include transient operating conditions and reflect reality much better.

For the purpose of this thesis, the final hierarchy of data selection from literature sources was fixed. The most valuable were the results from the latest WLTC procedure, next NEDC, then not legislated measurements. The lowest priority gained steady state conditions due to limitations described above.

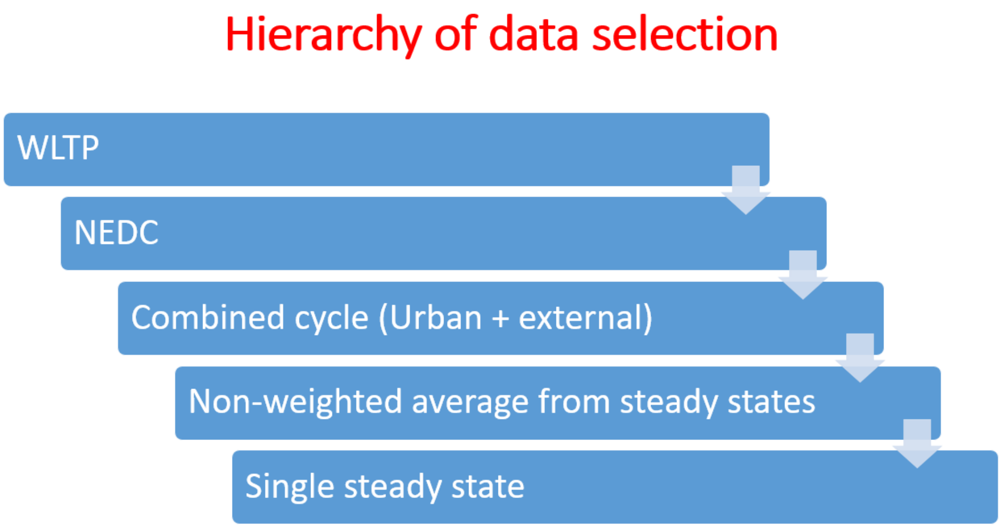


Figure 34: Importance of selected data for purpose of this work.

4.5.1 NEDC

New European Driving Cycle (NEDC) is a test for emissions and fuel consumption approval. It was devised for light-duty vehicles and established in a purpose of legislation in the European market in the year 2000. The measurement is done on a chassis dynamometer and it is divided into 2 sections: Urban Driving Cycle (UDC) and Extra Urban Driving Cycle (EUDC). The first section represents city center driving conditions with low speed and low load whereas the second one reflects driving on the highway with high speed. The NEDC test, lasting 1180 seconds, consists successively of four UDC repetitions (each 195 s) and one run of EUDC (400 s) without any interruption. Total distance covered is 10.93 km, average speed 33.35 km/h and maximum speed 120 km/h [45]. The schematic of NEDC speed profile is presented in Figure 35.

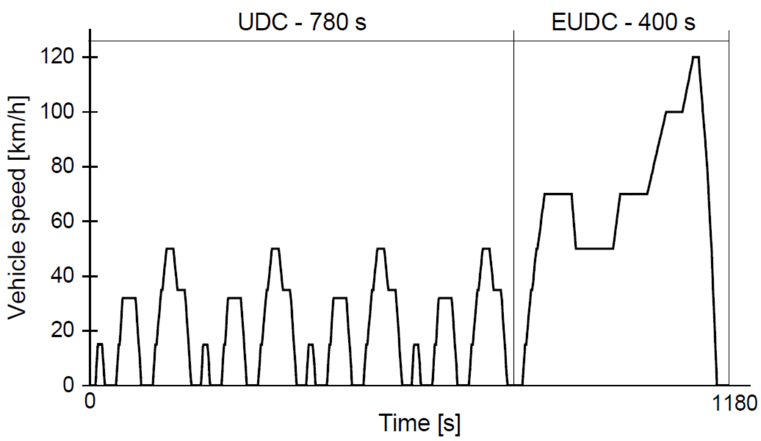


Figure 35: NEDC test procedure [46].

4.5.2 WLTC

Worldwide Harmonized Light Vehicles Test Cycle (WLTC) is a part of Worldwide Harmonized Light Vehicles Test Procedures (WLTP). Beside WLTC also Real Driving Emissions (RDE) are covered by the WLTP. Currently, WLTC is replacing NEDC procedure. The reason behind the aforementioned shift is a fact that NEDC is designed for former traffic and engine conditions. Nowadays, the end-user behavior and engine specification changed and that is why NEDC is not reflecting reality in the best possible way. The main difference is a wider range of engine operational points included in the test. It means that instead of modular speed profile, it is more diversified and dynamic when comparing to NEDC [47]. Nevertheless, WLTC has still the same purpose as NEDC and is performed on a chassis dynamometer. The test speed profile is shown in Figure 36.

Worth mentioning is fact that WLTC is divided into different classes in respect to the type of the light-duty vehicle. Class 3b is the most applicable for EU market as it encompasses highest power-to-weight ratio vehicles with a maximum speed over 120 km/h [48]. The duration time is extended to 1800 seconds when comparing with NEDC and distance covered equals 23.27 km. Also, maximum and average speed are elevated in order to better reflect real driving conditions than NEDC.

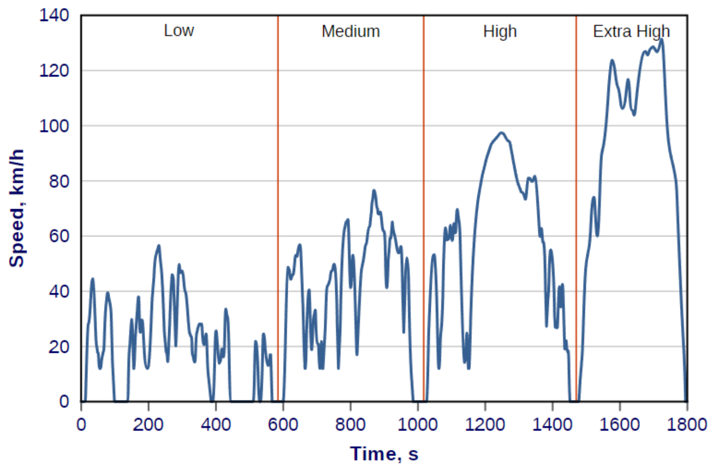


Figure 36: WLTC test procedure for class 3b passenger car [48].

4.5.3 Literature sources

In order to create uniform and representative model, reliable data are the crucial thing. Analysis of fuel property impact on engine performance requires plausible measurement results. In a case of ICE, the experimental set-up really plays a significant role. It creates the main task of the thesis very complex and demanding, especially when it comes to acquiring test data from other researches. Highest priority have measurements made on different blends of alternative fuels with various blending ratios. After the long searching process, the most promising articles were selected. Among them, the most important are SAE papers and IEA AMF report.

Also, thanks to the kindness of Andrzej Szczotka and Joseph Woodburn, researchers at BOSMAL Automotive Research and Development Institute Ltd in Bielsko-Biala in Poland, valuable papers written in that institute were included in the analysis. The initial articles for the purpose of modeling are shortly described below.

1. Source: Kim, D., et al. *Engine performance and emission characteristics of hydrotreated vegetable oil in light duty diesel engines.*, Fuel 2014. [49]

   Three types of fuels were analyzed and compared to standard diesel. Biodiesel used in the study consists of FAME produced 80% from palm-based oil and 20% from waste cooking oil (WCO). HVO is based on crude palm oil and iso-HVO was produced by process of isomerization of HVO. The results of fuel consumption are presented for following blends of each fuel: 2%, 10%, 20%, 30% and 50%. All fuel properties were extracted from this paper [49].

	Engine specification
1	**1.5 CRDI** from 2006, 4c
	CR = **17.8**
	b/s = 75/85
	DI, turbocharger, common-rail
	EGR, DOC, without DPF
	Euro 3 compliant
	Tests run on **NEDC**
	South Korea, 2014 (Fuel)

2. Source: Prokopowicz, A., et al. *The effects of neat biodiesel and biodiesel and HVO blends in diesel fuel on exhaust emissions from a light duty vehicle with a diesel engine.*, Environmental Science and Technology, 2015. [34]

   Blends of rapeseed biodiesel and HVO were analyzed and compared to standard diesel. Pure RME was provided by PKN Orlen whereas HVO by Neste. The results of fuel consumption and emissions performed on chassis dynamometer were presented for following blends of RME: 7%, 15%, 30% and 100%. There was only one HVO blend: 30%. Fuel properties such as density, viscosity and lower heating value were extracted from this literature source [34], the same applies to cetane number, except HVO blend - it was taken from [50]. Oxygen content was estimated based on [51].

	Engine specification
2	**1.9L JTD** from Fiat Croma 2009, 4c
	CR=**17.5**
	b/s = 82/90.4
	DI, turbocharger, common-rail
	EGR, DOC, without DPF
	Euro 4 compliant
	Tests run on **NEDC**
	Poland, 2015 (ACS)

3. Source: Birzietis, G., et al. *Effect of commercial diesel fuel and hydrotreated vegetable oil blend on automobile performance.*, Agronomy Research, 2017. [52]

   The main aim of this study was to compare the fuel consumption of fossil-based diesel with HVO blended diesel fuel from Neste in a specially designed driving cycle. Only one blend examined - 10% HVO blend. All properties were taken from this source [52], except LHV (from [53]).

	Engine specification
3	**2.2L** from Mazda CX 2015, 4c
	CR = **14.0**
	DI, common rail
	Euro 6 compliant
	IM-240 : **combined driving cycle**
	Latvia, 2017 (Agronomy Research)

4. Source: Omari, A., et al. *Improving Engine Efficiency and Emission Reduction Potential of HVO by Fuel-Specific Engine Calibration in Modern Passenger Car Diesel Applications.*, SAE International Journal of Fuels and Lubricants, 2017. [36]

   Pure HVO was tested according to WLTC procedure. Performance of alternative fuel was compared with standard diesel. Also, optimization of the engine was investigated. HVO was provided by Neste and all properties extracted from this source [36], except viscosity, which values were taken from *Neste Renewable Diesel Handbook* [53].

	Engine specification
4	**1.6L**, 4c
	CR=**17.0** (two-stage: 14 and 17)
	b/s=75/88
	DI, common-rail, 2-stage turbo
	EGR, DOC, DPF
	Euro 6 compliant
	WLTP tests
	Germany/Finland, 2017 (SAE)

5. Source: Millo, F., et al. *Experimental investigation on the effects on performance and emissions of an automotive Euro 5 diesel engine fuelled with B30 from RME and HVO.*, SAE Technical Paper, 2013. [54]

   Three fuels were analyzed: standard diesel, RME 30% blend and HVO 30% blend. Seven steady points were selected as representatives of NEDC, then fuel consumption and emissions estimated based on weighting scheme from [55]. All fuel properties were extracted from this literature source [54].

	Engine specification
5	**1.25L** with in-line 4c
	CR=**16.8**
	b/s=70/82
	DI, turbocharger, common-rail
	Euro 5 compliant
	Tests run on **NEDC**
	Italy, 2013 (SAE)

6. Source: Armas, O., et al. *Impact of animal fat biodiesel, GTL, and HVO fuels on combustion, performance, and pollutant emissions of a light-duty diesel vehicle tested under the NEDC.*, Journal of Energy Engineering, 2014. [56]

   Three pure alternative fuels were compared to standard diesel. Biodiesel was produced from animal fat and provided by BDP Company, GTL was produced by the Fischer-Tropsch process and supplied by SASOL. HVO fuel was provided by Neste and diesel fuel by CEPSA. NEDC tests were performed on chassis dynamometer for Nissan Qashqai. All fuel properties were extracted from this literature source [56].

	Engine specification
6	**2.0L dCI** Nissan Quashqai, 4c
	CR=**15.6**
	b/s = 84/90
	DI, turbocharger, common-rail
	EGR, DOC, DPF
	Euro 5 compliant (4)
	Tests run on **NEDC** (chasis)
	Spain, 2015, (J. Energy Eng.)

7. Source: Bermúdez, V., et al. *Comparative study of regulated and unregulated gaseous emissions during NEDC in a light-duty diesel engine fuelled with Fischer Tropsch and biodiesel fuels.*, Biomass and Bioenergy, 2011. [57]

Three types of 100% biodiesel and additionally 100% GTL were analyzed based on NEDC tests. The biodiesels were produced via transesterification and types included in the research were as follows: rapeseed, palm and soybean. GTL was produced by the Fischer-Tropsch process. All properties were given in that paper [57].

7	Engine specification
	2.0L HSDI (Citroen, Peugeot), 4c
	CR=18
	DI, turbocharger, common-rail
	EGR
	Euro 4 compliant
	Tests run on NEDC
	Spain, 2011, (Biomass and Energy)

8. Source: Napolitano, P., et al. *Hydrocracked Fossil Oil and Hydrotreated Vegetable Oil (HVO) Effects on Combustion and Emissions Performance of "Torque-Controlled" Diesel Engines.*, SAE Technical Paper, 2015. [55]

Four specific fuels were analyzed and compared with standard diesel based on steady state measurements and weighting formula in order to obtain NEDC results. Standard diesel fuel, diesel with streams from the hydrocracking process (Hck), Hck with 15% HVO blend, Hck with 30% HVO blend and Hck with cetane improver were tested. All fuel properties extracted from this source [55].

8	Engine specification
	2.0L , 4c
	CR=16.5
	b/s = 83/90
	DI, turbocharger, common-rail
	EGR, DOC, DPF
	Euro 5 compliant
	Tests run on NEDC
	Italy, 2015, (SAE)

9. Source: Karavalakis, G., et al. *Regulated and unregulated emissions of a light duty vehicle operated on diesel/palm-based methyl ester blends over NEDC and a non-legislated driving cycle.*, Fuel, 2009. [58]

Palm-based methyl ester blends of 5%, 20% and 40% were examined. Such biodiesel blends were tested on a chassis dynamometer with Toyota Hilux car. Viscosity, density and cetane number were extracted from that source [58] while LHV and oxygen content from [35].

9	Engine specification
	2.5L TD (Toyota Hillux), 4c
	CR=18.5
	b/s = 92/94
	DI, turbocharger, common-rail
	DOC
	Euro 3 compliant
	Tests run on NEDC
	Greece, 2009, (Fuel)

10. Source: Stengel, B., et al. *Synthesis, Characterization, and Use of Hydro-Treated Oils and Fats for Engine Operation.*, IEA AMF, 2015. [43]

HVO, standard FAME and enzymatic FAME (E-FAME) were examined and compared with diesel. Standard FAME obtained by transesterification while E-FAME was produced with the use of special enzymes. Measurements for steady states were converted to NEDC via formula from [55]. All properties in detail examined in the project and included in Annex [43].

10	Engine specification
	2L , VW Passat, 4c
	CR=18.5
	b/s=81/96
	DI, common-rail, turbocharger
	EGR, DOC, DPF, SCR
	Euro 6 compliant
	multiple steady-state tests
	Germany/Denmark, 2015 (IEA AMF

4.6 Mathematical modeling

This section presents modeling methods used to obtain the main goal of the thesis described in Section 2. The final approach of the task is presented in Figure 37. In principle, the blend is determined by volume concentration of alternative fuel ($\%X$) while the rest is standard diesel ($\%Y$). Such a specified blend owns well-measured properties (A, B, C, D). In addition, for that specific blend, the engine performance is also provided by the test data (α, β, γ, δ). However, the impact of every single property on final engine performance is unknown. That is exactly what model should indicate as a final outcome. Moreover, the model is going to predict final performance based only on provided fuel properties (i.e. by fuel producer), regardless of the fuel blend type. After observations from literature, it was noticed that blending rate affects final properties of the mixture. In addition, blending ratio influences engine performance. Nevertheless, the contribution of single property on performance is not directly known. The final model should indicate, which properties matter the most and to what extent they impact i.e. fuel consumption.

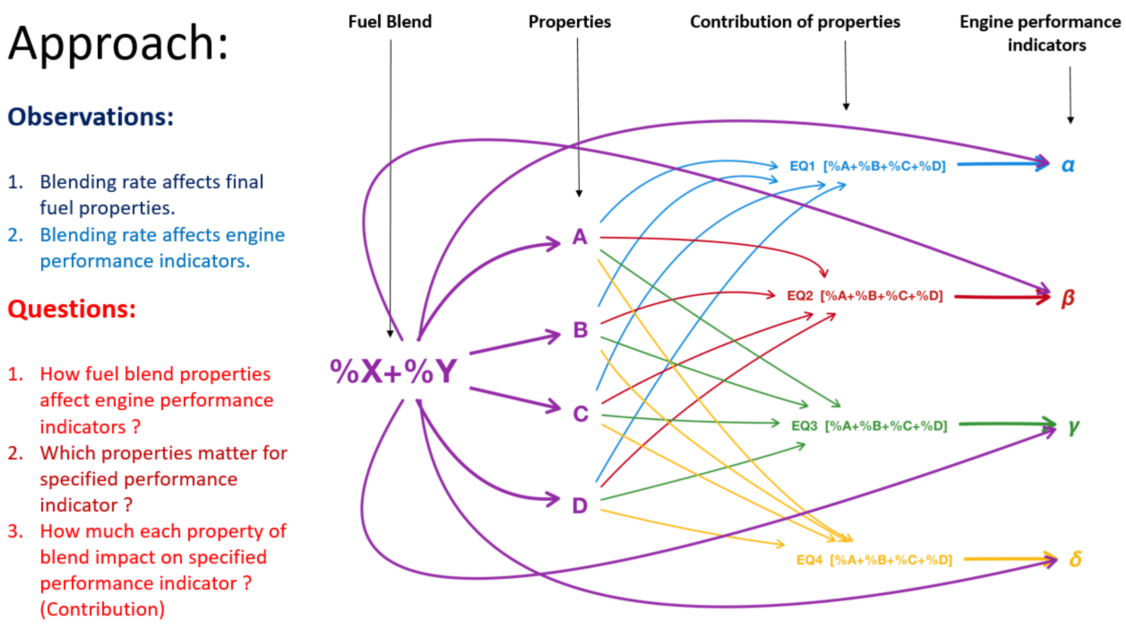


Figure 37: Graphically presented final modeling approach.

Selection of mathematical method was the next step after determining final approach described above. Having various data from other researches, an appropriate technique of analysis was needed. After careful consideration and initial data analysis, multilinear regression was selected. It was decided that parameters in terms of fuel properties (identified in Section 4.3) would be used as multiple inputs for modeling. The engine performance was designated as a single output and fuel consumption as a representative indicator was taken into account. All the modeling data could be gathered inside a matrix utilized in multilinear regression procedure. In general, any linear relationship can be expressed by Equation [59]:

$$y(x) = \phi_1(x) \cdot \theta_1 + ... + \phi_n(x) \cdot \theta_n \tag{4.6.1}$$

or in matrix form:

$$y = \phi \cdot \theta \tag{4.6.2}$$

where,
y - dependent observable variable;
x - independent variable;
$\phi_1(x)...\phi_n(x)$ - explanatory variable;
$\theta_1...\theta_n$ - parameter corresponding to consecutive explanatory variable.

For the purpose of this work, the equation 4.6.1 can be rewritten in a form presented below.

$$\alpha = a \cdot A(X) + b \cdot B(X) + c \cdot C(X) + d \cdot D(X) + e \cdot E(X) \tag{4.6.3}$$

where,
X - alternative fuel volumetric concentration in fuel blend;
α - fuel consumption (in respect to l/km);
$A(X)...E(X)$ - fuel property value dependent on concentration;
$a...e$ - parameter corresponding to each consecutive fuel property.

In the given task, the parameters $a...e$ were unknown and estimated by the means of the least-square method described in detail in sources [59], [60]. Regression was executed in OriginLAB software, where coefficients were monitored [61]. The algorithm used to solve the problem was Levenberg-Marquardt. However, it is important to note that various properties are interrelated. Initial multilinear regression was followed by single linear regression for LHV. The procedure is similar to multilinear regression but only one single input is analyzed. LHV volumetric-based was selected as a property, which is the most influential on fuel consumption. The anticipated direct proportional correlation between FC and LHV was examined. Obtained coefficient was after that used in the final multilinear regression as a fixed parameter.

Before creating a final matrix, the uniform method for presenting data was crucial. Raw numerical data from different researches are hard to compare. Especially specific fuel consumption and emissions are highly dependent on engine type. However, there was proposed one plausible solution. It was based on the observation that in all analyzed literature sources alternative fuel blends were examined but always measurements for standard fossil-based diesel were performed, too. Therefore, it was decided to express all the results by relative changes. This approach with relative changes was applied both to fuel properties and engine performance indicator. All raw numerical data were converted to percentage changes referred to standard diesel and its performance. Executed procedures, before completing final matrix of input and output data, are listed below.

- Fuel properties are expressed in relative (%) changes - a reference to standard diesel.
- Engine performance indicators also are expressed in relative changes (%) compared with the performance of reference fuel.
- Model is going to present the percentage change (increase or decrease) in fuel consumption (in respect to l/km) and emissions (in respect to g/km) dependent on the percentage change of fuel properties.

CO_2 emission prediction is based on results from multilinear regression for fuel consumption. Knowing the fuel consumption per 100 km, the CO_2 emissions per 1 km can be calculated. However, essential is knowledge of carbon content in the fuel blend. For pure fuels the values are obtained automatically but for blends additional calculation should be carried out - Equation 4.6.5. Finally, knowing the values of density, it is enough to obtain the result by Equation 4.6.4.

$$\beta = \alpha \cdot \rho \cdot z \cdot 44/12 \tag{4.6.4}$$

where,
β - CO_2 emissions;
α - fuel consumption;
ρ - density of the fuel blend;
z - carbon content [mass based] in a fuel blend.

$$z = (x \cdot z_a \cdot \rho_a + (1 - x) \cdot z_d \cdot \rho_d)/\rho_b \tag{4.6.5}$$

where,
x - volumetric fraction (concentration) of alternative fuel;
ρ_a - density of pure alternative fuel;
ρ_d - density of standard diesel;
ρ_b - density of final fuel blend;
z_a - carbon content in alternative fuel;
z_d - carbon content in standard diesel fuel.

4.6.1 Quality of the model

Quality of fitting is examined by checking various parameters such as adjusted R-square, standard error, t-value. The validation of the model is done by residual analysis and cross-validation technique [60]. A residual analysis shows the predictions error when comparing theoretical values with those obtained from the model - Equation 4.6.6.

$$y(x) = \phi(x) \cdot \theta - \epsilon(x) \tag{4.6.6}$$

where,
x - independent variable;
$y(x)$ - observable output;

$\phi(x)$ - explanatory variable;
θ - parameter (coefficient);
ϵ - error of prediction.

Prediction errors are estimated by scalar function, which is minimized. Hence, it is called the least-square method described by the Equation 4.6.7 ([59]).

$$J_\theta = \sum_{x=1}^{N} \epsilon^2 = \sum_{x=1}^{N} (y(x) - \phi^T(x) \cdot \theta) \tag{4.6.7}$$

where,
J_θ - least-squares objective function.

Other quality measurement is a cross-validation technique. It means that the whole set of data is divided into two groups. One group is used as input data for fitting and model development. Another group is used for checking the correctness of the outcome.

In this project, both residual and cross-validation were proceeded on the collected data in order to examine the quality of the final model. However, it should be remarked that the final outcome is highly influenced by the input data obtained from the available literature. It should be also taken into account that *the result of the modeling process can be no better than what corresponds to the information contents in the data.* [60]. In the ideal case, external data from commercial sector could be used for final validation and further improvements of the model.

4.6.2 Key modeling steps

Modeling main points are listed below.

1. All values of fuel properties and engine performance converted to relative changes.
2. The character of the data: multiple inputs, single output.
3. Creating a final matrix with selected fuel properties as input and engine performance as output.
4. Mathematical methodology: multilinear regression.
5. Iteration algorithm: Levenberg-Marquardt.
6. Coefficients optimization process.
7. Validation and sensitivity analysis.
8. Final model proposal.

5 Results

5.1 Steady state approach

After an extensive review of publicly available scientific articles, it turned out that final performance of an engine is highly dependent on its load and speed. In addition, different engines and measurement set-ups express in various results and lead sometimes to inconsistency. Observations from literature showed many limitations when considering only steady state operating conditions. Certainly, an obstacle is interference of both engine and fuel influence while considering final performance.

When examining fuel property impact on engine performance, main observations from extensive literature review were collected below.

- In literature, there is a lot of articles with measurement data. Inconsistency in nomenclature can be observed. Even in *Fuel* paper from 2010, the author names tested fuel as RME biodiesel [62]. In fact, it is just straight vegetable oil (SVO). There is also a lot of contradictory results in the literature, a good example is a biodiesel. Reviews such as [44],[63],[64],[65] indicate those discrepancies, i.e. in some cases, BTE drops while in others grows. Here comes the question, which data can be treated as the most reliable and representative.

- In order to make a database, there is a need for extraction of data from different sources such as articles, publications and journal papers. The measurements are carried out in various parts of the globe and standard diesel fuels own different properties. In addition, fuels are tested in miscellaneous engines, starting from small ones and finishing on big ones, also with changeable configuration (single-cylinder/multiple-cylinder, total displacement, compression ratios specific for each engine). That is why it is hard to compare final results, even though the aims of researches are the same. Combining multiple sources and obtaining data is essential for creating a model.

- It should be taken into account that engine performance is not only influenced by the fuel properties, but it is also dependent on the load, engine speed or driving conditions in general. Type of engine/vehicle has an impact, too.

- There is a limited access to full spectrum of data, meaning that the volume concentration of alternative fuel rarely changes from 0 up to 100% in blends. Usually, measurements are denser in the range 0-30% - especially second half of blend range (50-100%) needs approximation by interpolation or extrapolation, in most cases, the linear approach seems to be sufficient. However, sometimes a specific behavior of the property or engine performance can be lost for in-between range when measurements are kept less frequently.

- Fuels are characterized by plenty of properties, some of them are given by norms (i.e. EN 590). But some are not specified by standards, such as autoignition temperature, LHV. For the modeling purposes, there is a need for appropriate selection of the most significant properties affecting the engine performance.

- Not all properties should be considered as independent variables, there are some dependent variables, which can be coupled, i.e. LHV and density (into volumetric LHV).
- Moreover, fuel properties can be considered to influence the engine performance by altering the combustion characteristics. Hence, fuel might be perceived to impact engine performance indirectly through such parameters as ignition delay, HRR. Nevertheless, this approach makes the task even more complicated.
- The final task is a really complex issue, it combines fuels and fuel properties with the engine and its operational conditions.

After observations and conclusions from literature review, the analysis of steady state approach in two steps is conducted. The first step encompasses comparison of results from selected sources 'A', 'B', 'C' and 'D' described in Section 4.4. The graphical presentation is shown in Figure 38. Relative changes of fuel consumption are applied on Y axis whereas on X-axis RME volumetric concentration is indicated. Even in case of those most promising researches, a visible discrepancy is observed and it could be justified by different measurement set-up configurations and not corresponding operating conditions. From such a database it is extremely hard to extract some universal behavior. In article 'B' the BSFC slightly increases while in source 'A' significant growth is observed. Moreover, in paper 'D' there is some particular behavior noticed - for 10% blend, the BSFC is the lowest and in higher concentrations, it rapidly increases. Based on such a data, there is no possibility to create a general and uniform model.

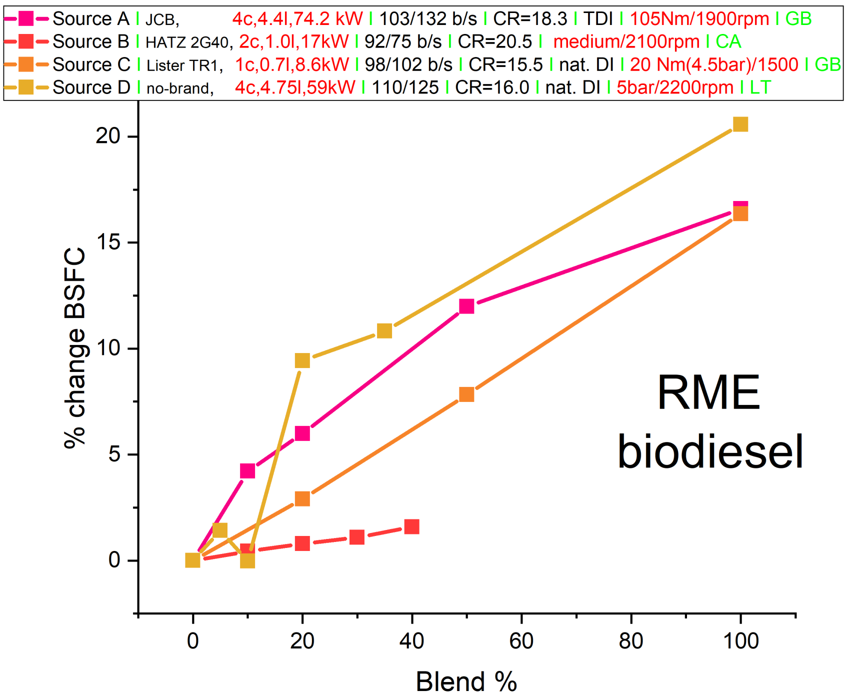


Figure 38: Results of BSFC relative changes in different researches.

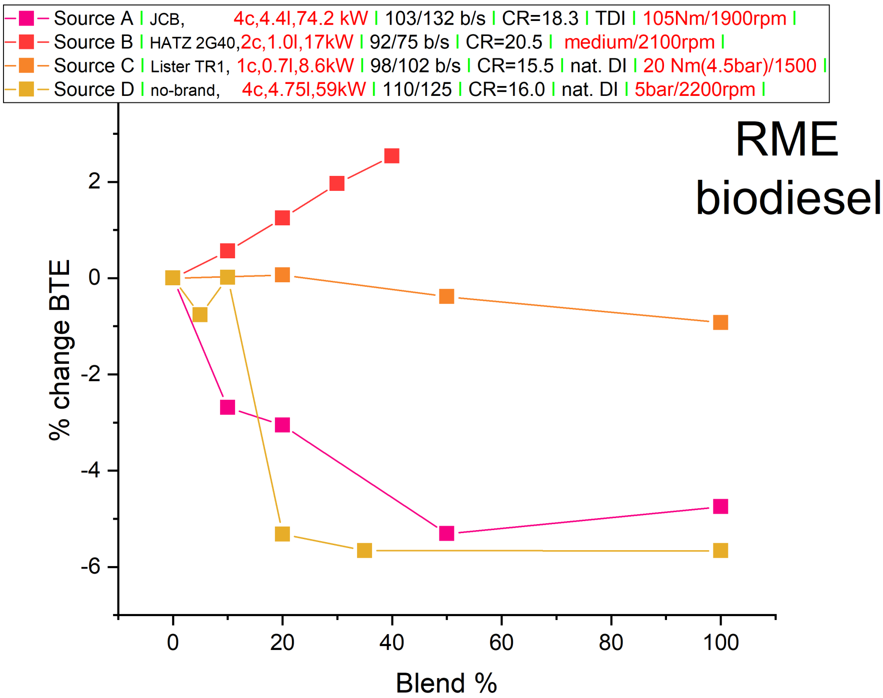
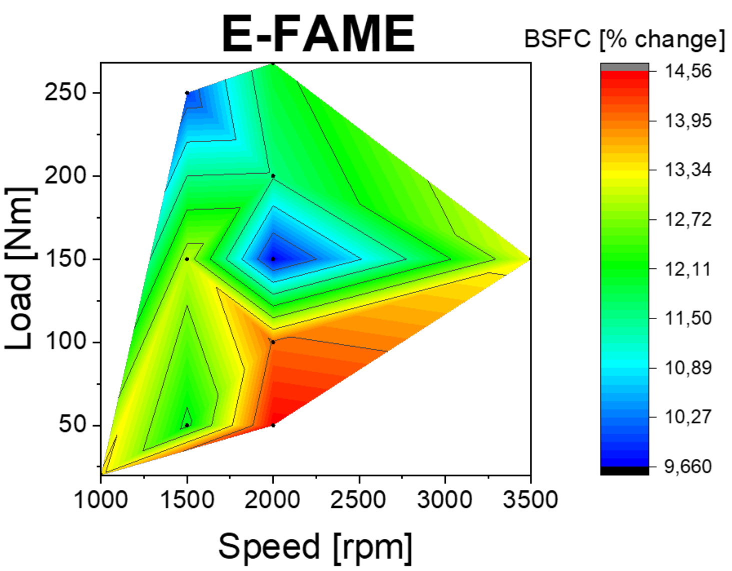


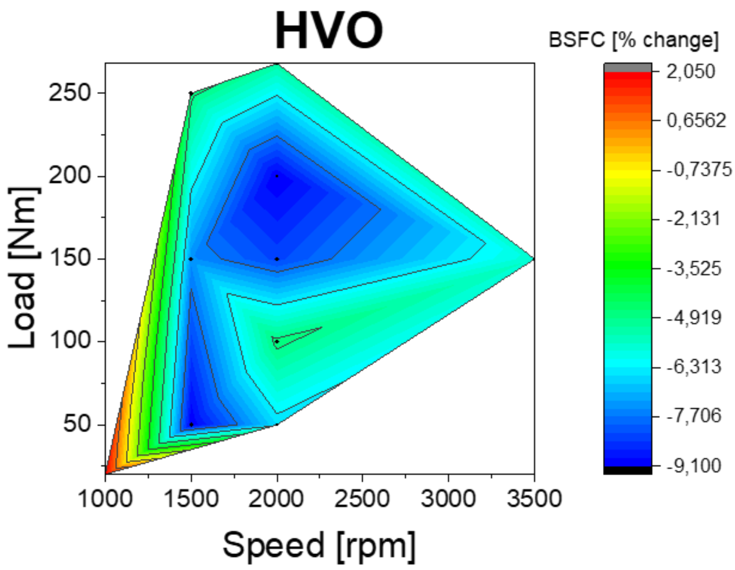
Figure 39: Results for the same fuel blends but from different measurements available in literature - BTE relative changes.

Not only BSFC measurements are deviating a lot. Even more significant discrepancies are observed for brake thermal efficiency when considering the same literature sources. In Figure 39 the BTE results are presented. In source 'B' with an increase of blending ratio, the growth of BTE is observed. In contrary, for source 'A' significant drop is monitored, whereas for source 'C' almost no changes are reported. For research 'D' there is a peculiar behavior for low blending ratios.

The second step of steady state analysis included an examination of IEA AMF project results. The measurements were done on modern diesel engine complying with EURO VI norms. Engine operational maps for two different fuels in terms of fuel consumption are compared in Figure 40. Those are three-dimensional plots with X-axis denoting engine speed, Y-axis load and colors represent relative change in fuel consumption in reference to standard diesel. From the analysis of those maps, it becomes obvious that engine operational conditions matter a lot. They have a very significant influence on final performance. In a case of HVO, fuel consumption for idling mode is slightly increased (+2%) when comparing to standard diesel. The opposite effect is observed for high speed and high load conditions (-5%). Moreover, for moderate operating conditions significant reductions in fuel consumption are observed (up to -9%). For E-FAME the fuel consumption is increased in all cases but the extreme values range from 9,5% to 14,5%, for standard FAME the variations are even more visible (from 8 to 20% growth in BSFC when comparing with standard diesel). The similar particular behavior occurs for specific emissions of NO_x, what is reported in IEA AMF annex [43].



(a) BSFC for E-FAME fuel.



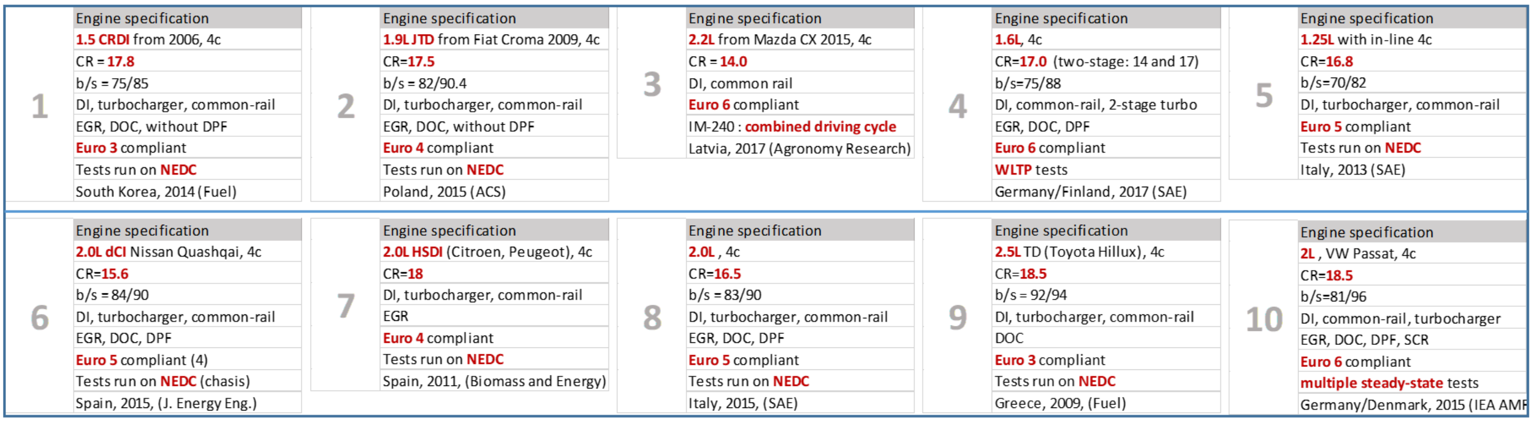
(b) BSFC for HVO fuel.

Figure 40: Relative changes of BSFC in reference to standard diesel fuel. Based on data from IEA AMF project [43].

Extensive literature review and two steps of steady state analysis presented above contributed to reshaping the initial approach. Summary of important observations influencing switching from steady state analysis into driving cycle procedures is presented in points below.

- Careful data selection crucial for model quality.
- Test engine specifications are very significant. More valuable are measurements on the representative engine instead of experimental non-commercial set-up.
- Engine operation conditions have a huge impact on how fuel properties affect engine performance.
- Having data from measurements in full spectrum of engine's operational conditions still does not guarantee general conclusions and unambiguous interpretation.
- Driving cycles, which are weighted average from steady states could mitigate the influence of the engine on final performance.
- While real driving, there are many transient conditions, which cannot be represented by steady state operation.
- Test mode (steady state conditions or driving cycle test procedure) is very important. From the end-user point of view, the driving test procedures are much more representative when considering passenger cars.

5.2 Driving cycle test procedures



1	2	3	4	5
Engine specification	Engine specification	Engine specification	Engine specification	Engine specification
1.5 CRDI from 2006, 4c	1.9L JTD from Fiat Croma 2009, 4c	2.2L from Mazda CX 2015, 4c	1.6L, 4c	1.25L with in-line 4c
CR = 17.8	CR=17.5	CR = 14.0	CR=17.0 (two-stage: 14 and 17)	CR=16.8
b/s = 75/85	b/s = 82/90.4	DI, common rail	b/s=75/88	b/s=70/82
DI, turbocharger, common-rail	DI, turbocharger, common-rail	Euro 6 compliant	DI, common-rail, 2-stage turbo	DI, turbocharger, common-rail
EGR, DOC, without DPF	EGR, DOC, without DPF	IM-240 : combined driving cycle	EGR, DOC, DPF	Euro 5 compliant
Euro 3 compliant	Euro 4 compliant	Latvia, 2017 (Agronomy Research)	Euro 6 compliant	Tests run on NEDC
Tests run on NEDC	Tests run on NEDC		WLTP tests	Italy, 2013 (SAE)
South Korea, 2014 (Fuel)	Poland, 2015 (ACS)		Germany/Finland, 2017 (SAE)	

6	7	8	9	10
Engine specification	Engine specification	Engine specification	Engine specification	Engine specification
2.0L dCI Nissan Quashqai, 4c	2.0L HSDI (Citroen, Peugeot), 4c	2.0L , 4c	2.5L TD (Toyota Hillux), 4c	2L , VW Passat, 4c
CR=15.6	CR=18	CR=16.5	CR=18.5	CR=18.5
b/s = 84/90	DI, turbocharger, common-rail	b/s = 83/90	b/s = 92/94	b/s=81/96
DI, turbocharger, common-rail	EGR	DI, turbocharger, common-rail	DI, turbocharger, common-rail	DI, common-rail, turbocharger
EGR, DOC, DPF	Euro 4 compliant	EGR, DOC, DPF	DOC	EGR, DOC, DPF, SCR
Euro 5 compliant (4)	Tests run on NEDC	Euro 5 compliant	Euro 3 compliant	Euro 6 compliant
Tests run on NEDC (chasis)	Spain, 2011, (Biomass and Energy)	Tests run on NEDC	Tests run on NEDC	multiple steady-state tests
Spain, 2015, (J. Energy Eng.)		Italy, 2015, (SAE)	Greece, 2009, (Fuel)	Germany/Denmark, 2015 (IEA AMF

Figure 41: All analyzed literature sources summary.

Articles described in Section 4.5 provided necessary data for analysis. Summary of technical specification used in each research is presented in Figure 41. The information about fuel properties and consumption were extracted from aforementioned sources and then numerical data converted to relative changes in reference to standard diesel. After that stage, the dependency of fuel consumption from the single property was plotted combining data from all available sources. One of the outcomes is presented in Figure 42. The notation of labeling in following figures consists of three parts. First part - the number denotes source (1-10); second part - the text represents fuel (B - biodiesel, H - HVO, Be - enzymatic biodiesel, Hi - isomerized HVO, GTL, FT - Fischer-Tropsch diesel, Hck - diesel with streams from hydrocracking process.); third part - the number specifies the volumetric concentration of alternative fuel in a blend.

After second in-depth review of all 10 sources and initial data analysis, it was decided to reject from modeling three sources: 3, 7, 9. The reasons are presented below. The outcome of such a modification results in more consistent data shown in Figure 43.

Rejected from modeling:

- Source 3: This research presents results not from NEDC test but from the specially designed driving procedure. The main drawback is a fact that the distance covered in this test is significantly shorter than for NEDC - only 3 *km*.
- Source 7: The values of properties and results exhibit significant deviations from all other sources. In particular, the inconsistency can be seen when comparing Figures 42 and 43.
- Source 9: It was the oldest research and article was published in 2009. Moreover, the engine is bigger than in case of other sources.

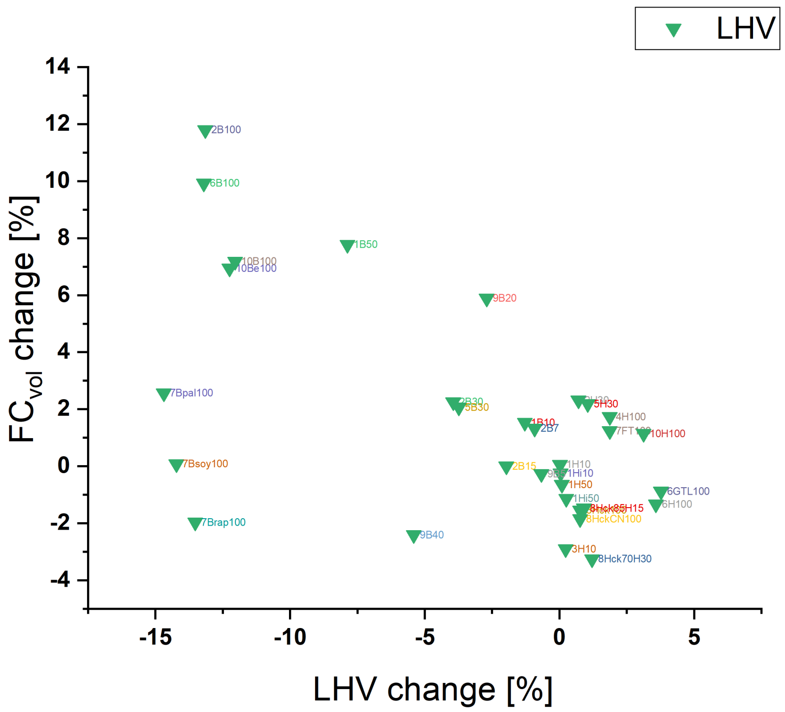


Figure 42: Dependency of fuel consumption from LHV for all 10 sources.

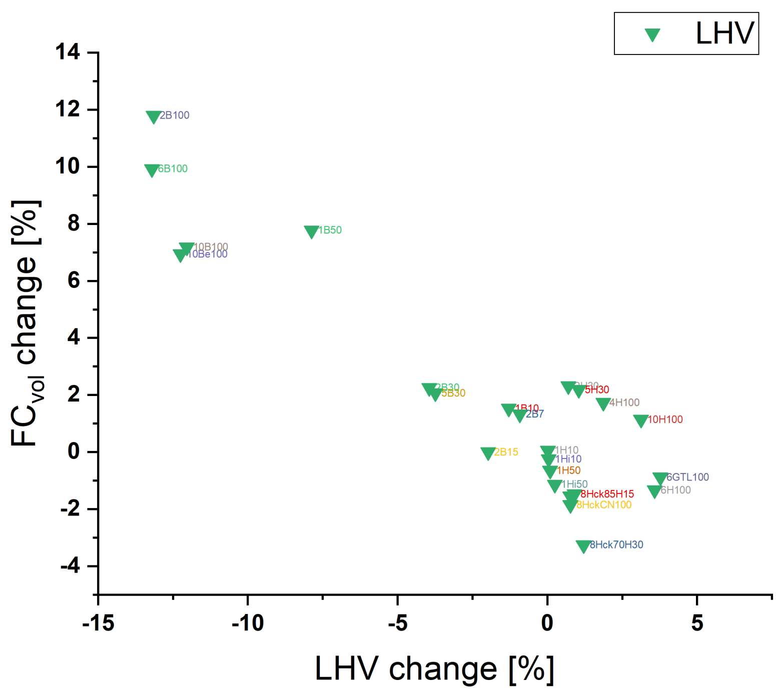


Figure 43: Final 7 analyzed literature sources - dependency of FC from LHV.

According to the final selection, it turned out that only the newest articles were taken into account from years 2013-2017. Such a data seem to be the most reliable and have a potential to reflect reasonably the recent market situation. Owning data mostly from NEDC test procedure, it was possible to create the final matrix necessary for multilinear regression. Additionally, weights of the measurements points were established in order to have the same contribution from each source. The final matrix utilized for purpose of multilinear regression is presented in Figure 44. Input parameters are density, viscosity, cetane number, volumetric LHV and oxygen content. The output is specified by fuel consumption. All values of input and output parameters represent relative changes with reference to standard diesel fuel (except oxygen content, which is presented based on mass concentration in a blend). The numerical values from matrix can be visualized and it is done in Figure 45.

Fuels for Compression Ignition Engines								
		MULTIPLE INPUT					WEIGHT	SINGLE OUTPUT
		Properties						Engine Performance Indicator
		Density	Viscosity	CN	LHV vol	Oxygen		Fuel Consumption
		% CHANGE						% CHANGE
SOURCE	FUELS	A	B	C	D	E	WEIGHT OF THE POINT	Alpha
	Diesel	0,00	0,00	0,00	0,00	0,00	1,00	0,00
1	B10	0,61	5,28	2,71	-0,70	1,06	1,00	1,53
1	B20	1,21	12,20	4,45	-1,36	2,12	1,00	1,85
1	B30	1,94	19,92	6,19	-2,31	3,18	1,00	3,97
1	B50	3,16	34,55	7,54	-4,96	5,30	1,00	7,77
1	H10	-0,61	2,85	9,67	-0,58	0,00	1,00	0,06
1	H20	-1,09	5,28	19,34	-1,06	0,00	1,00	-0,07
1	H30	-1,58	8,54	27,66	-1,50	0,00	1,00	-0,35
1	H50	-2,55	14,63	37,14	-2,45	0,00	1,00	-0,64
1	Hi10	-0,61	1,63	8,32	-0,56	0,00	1,00	-0,25
1	Hi20	-1,21	3,66	14,31	-1,11	0,00	1,00	-0,30
1	Hi30	-1,94	6,91	21,86	-1,75	0,00	1,00	-0,76
1	Hi50	-2,67	10,16	26,50	-2,42	0,00	1,00	-1,13
2	B7	0,24	0,19	0,11	-0,68	0,74	2,00	1,33
2	B15	0,72	6,74	0,24	-1,27	1,59	2,00	0,00
2	B30	1,32	19,01	0,49	-2,68	3,18	2,00	2,26
2	B100	4,67	76,29	1,63	-9,09	10,60	2,00	11,80
2	H30	-2,39	3,99	17,75	-1,70	0,00	2,00	2,31
4	H100	-5,99	-16,67	49,53	-4,45	0,00	12,00	1,73
5	B30	1,85	18,72	3,13	-1,95	3,40	6,00	2,07
5	H30	-3,02	-5,07	18,55	-2,00	0,00	6,00	2,19
6	B100	3,79	60,56	21,03	-9,91	11,03	4,00	9,92
6	GTL100	-8,40	-6,77	64,58	-4,95	0,00	4,00	-0,88
6	H100	-7,69	19,12	74,91	-4,39	0,00	4,00	-1,33
8	Hck100	-0,06	11,79	0,76	0,71	0,00	3,00	-1,54
8	Hck85H15	-0,40	33,06	15,21	0,51	0,00	3,00	-1,47
8	Hck70H30	-1,07	49,57	30,04	0,13	0,00	3,00	-3,25
8	HckCN100	-0,06	11,79	22,62	0,71	0,00	3,00	-1,85
10	Be100	5,19	56,41	-2,26	-7,70	11,00	4,00	6,94
10	B100	4,43	67,28	14,88	-8,13	10,90	4,00	7,18
10	H100	-7,15	5,67	40,68	-4,25	0,00	4,00	1,14

Figure 44: Matrix of data with weights from final literature sources - dependency of FC from fuel properties - all values expressed in relative changes.

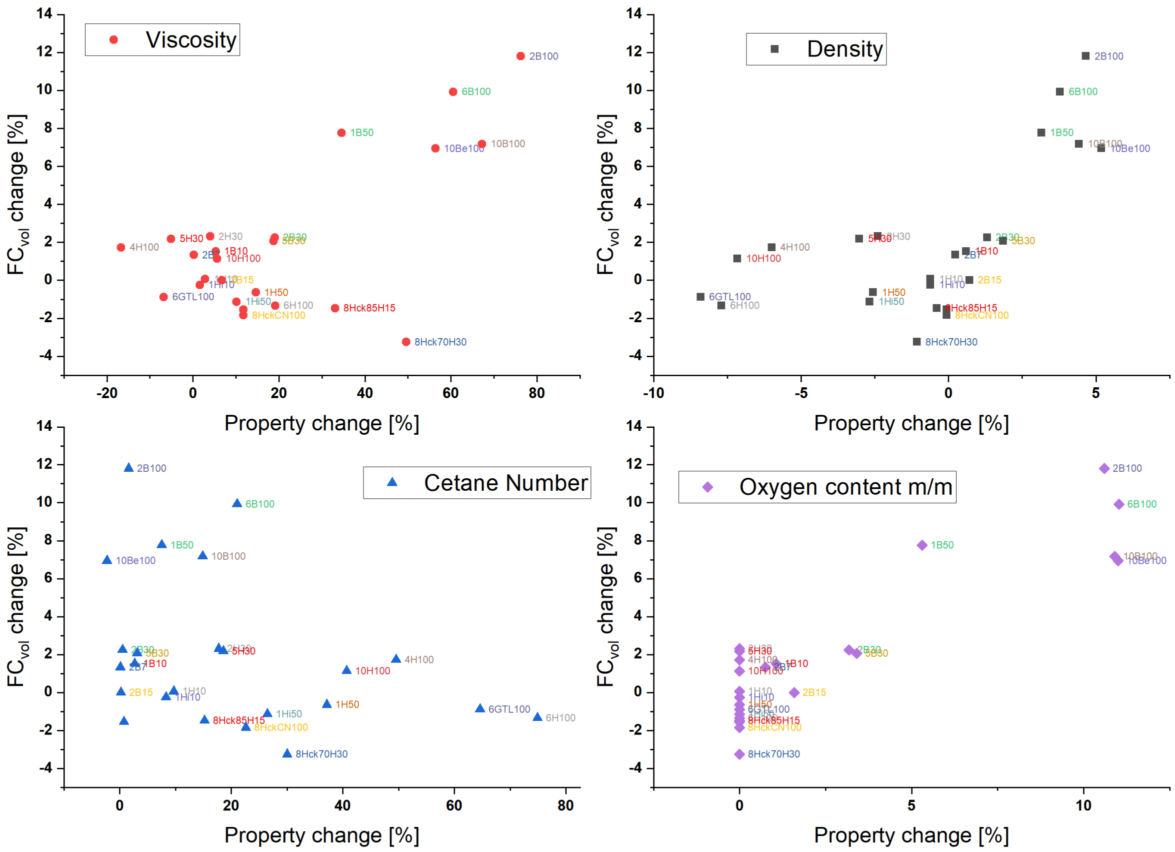


Figure 45: Dependency of fuel consumption from different properties combining 7 newest literature sources.

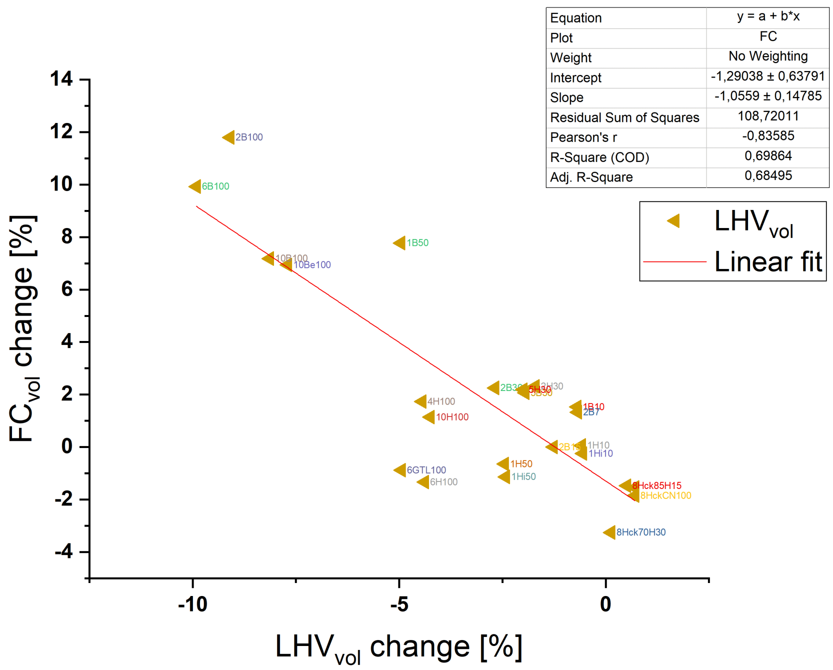


Figure 46: Dependency of fuel consumption from volumetric LHV - linear regression.

Proceeding with data collected in the matrix (Figure 44), multilinear regression was executed. However, the coefficient for lower heating value volumetric-based (changes related to MJ/l) was set as *-1*. The explanation of such an action can be justified as LHV is the main blend property, which impacts fuel consumption. In order to obtain the same power output, the injected volume of the fuel has to be changed proportionally to the shift of calorific value. Following the definition of LHV, it is intuitive that in a specified volume of liquid, there is a limited chemical energy collected, which can be further converted to useful mechanical work and power. According to the rule of thumb, the higher the LHV is, the less fuel is needed. Observation of results from different literature sources revealed a correlation between LHV and fuel consumption. The analysis presented in Figure 46 confirmed that there is a linear relation characterized by R-square equal 0,7 and Pearson's R equal -0,84. Moreover, the linear regression indicates directly proportional correlation with slope value very close to *-1*. For example, if 5% of decrease in LHV is observed, then approximately 5% increase in FC is expected. This straight relation between LHV and FC gave a reason to fix a parameter d in Equation 5.2.1 and set the value as *-1*. In order to examine the influence of other properties such as density, viscosity, oxygen content and cetane number, the multilinear regression method was proceeded and remaining coefficients fitted. The statistics of the parameters' fitting are presented in Table 11. The most important parameter is adjusted R-square, which eventually is equal 0,917 what makes the fitting satisfactory. Also, standard error of each coefficient is in the allowed range. Final model formula predicting fuel consumption based solely on properties is expressed by Equation 5.2.1. The equation includes coefficients obtained by multilinear regression (except LHV, which was obtained by single linear regression) and fuel properties are expressed in relative changes related to standard diesel fuel. The same applies to fuel consumption, the outcome of the model predicts if FC is increasing or decreasing for a given set of properties.

Coefficient	Value	Standard error	t-Value	Prob>ItI
a	0,155	0,128	1,214	0,228
b	-0,022	0,009	-2,312	0,023
c	-0,050	0,015	-3,319	0,001
d	-1,000	0,000	–	–
e	0,107	0,062	1,738	0,086

Table 11: Coefficients from multilinear regression.

$$\alpha = 0,155 \cdot A - 0,022 \cdot B - 0,050 \cdot C - 1,0 \cdot D + 0,107 \cdot E \tag{5.2.1}$$

α - relative change of fuel consumption (in respect to l/km);
A - relative change of density;
B - relative change of viscosity;
C - relative change of cetane number;
D - relative change of lower heating value;
E - relative change of oxygen content.

There are some very important observations from literature. Although the fuel blends have the same concentration of alternative fuel, differences in fuel consumption can be noticed when comparing various literature results. It is caused by different final fuel blend specification - concentration is the same but final properties are not the same. The model takes it into account and the validation for different fuels is presented in Table 12.

		Properties % change					FC_{vol} % change	
		Density	Viscosity	CN	LHV	O2	SOURCE	MODEL
B10	1B10	0,61	5,28	2,71	-0,70	1,06	**1,53**	**0,65**
	2B7	0,24	0,19	0,11	-0,68	0,74	**1,33**	**0,79**
	2B15	0,72	6,74	0,24	-1,27	1,59	**0,00**	**1,39**
B30	1B30	1,94	19,92	6,19	-2,31	3,18	**3,97**	**2,21**
	2B30	1,32	19,01	0,49	-2,68	3,18	**2,26**	**2,79**
	5B30	1,85	18,72	3,13	-1,95	3,40	**2,07**	**2,04**
B100	2B100	4,67	76,29	1,63	-9,09	10,60	**11,80**	**9,22**
	6B100	3,79	60,56	21,03	-9,91	11,03	**9,92**	**9,31**
	10BE100	5,19	56,41	-2,26	-7,70	11,00	**6,94**	**8,57**
	10B100	4,43	67,28	14,88	-8,13	10,90	**7,18**	**7,78**
H30	1H30	-1,58	8,54	27,66	-1,50	0,00	**-0,35**	**-0,32**
	2H30	-2,39	3,99	17,75	-1,70	0,00	**2,31**	**0,35**
	5H30	-3,02	-5,07	18,55	-2,00	0,00	**2,19**	**0,71**
	8Hck70H30	-1,07	49,57	30,04	0,13	0,00	**-3,25**	**-2,88**
H100	4H100	-5,99	-16,67	49,53	-4,45	0,00	**1,73**	**1,39**
	5GTL100	-8,40	-6,77	64,58	-4,95	0,00	**-0,88**	**0,54**
	5H100	-7,69	19,12	74,91	-4,39	0,00	**-1,33**	**-1,00**
	10H100	-7,15	5,67	40,68	-4,25	0,00	**1,14**	**0,97**

Table 12: Validation table.

Symbol	Property	Change [%]	Coefficient	Impact on FC_{vol} [%]
A	density	10	0,1549	+1,549
B	viscosity	-80	-0,02165	+1,732
C	CN	80	-0,0504	-4,032
D	LHV	-15	-1	+15
E	O2	12	0,10721	+1,28652

Table 13: Influence of single fuel property change on fuel consumption.

The contribution of single property can be associated with the corresponding coefficient used in the final equation. Table 13 demonstrates how single property impacts fuel consumption while other properties are kept constant - extreme allowable changes are taken into account. Finally, the cross-validation was executed. The multilinear regression was done excluding one literature source. Then the coefficients were compared with each other. This section shows that model is very sensitive with respect to input data. However, the coefficients vary in acceptable range, what means that model can be treated as universal.

Sources	All 7	Except 1	Except 2	Except 4	Except 5
Coefficient	Value	Value	Value	Value	Value
a	0,155	0,076	0,322	0,081	0,253
b	-0,022	-0,017	-0,035	-0,008	-0,023
c	-0,050	-0,059	-0,031	-0,065	-0,041
d	-1,000	-1,000	-1,000	-1,000	-1,000
e	0,107	0,111	0,062	0,073	0,064
Adj R-square	0,91716	0,92806	0,93364	0,92023	0,93099

Table 14: Comparison of coefficients for different multilinear regression results dependent on input data.

Additionally, pure DME fuel is tested on the model. Even though it is not a drop-in fuel and normally in gaseous form, the results are promising. It may be an implication of the fact that during injection DME is in liquid form and thus the nature of combustion is similar to standard diesel. The model indicates the significant increase in fuel consumption around 48,7% what is consistent with expectations [67]. In Table 15 significant fuel properties are presented, the data for DME are extracted from [66] while standard diesel specified in [36] is used as reference fuel.

Property	Density [kg/m3]	Viscosity [mm2/s]	CN	LHV [MJ/l]	O2 [%m/m]
Diesel	830	3,6	53,5	35,52	0
DME	660	below 1	55-60	19	35
Property change	A	B	C	D	E
Relative change [%]	-20,5	-90,3	7,5	-46,5	35,0

Table 15: Comparison of DME properties used for model testing.

CO_2 emissions are based on carbon balance. The results of fuel consumption are directly used in prediction of CO_2 emissions. For specified fuel blends it is important to know carbon content in pure fuels. The outcomes for few fuels are collected in Table 16.

Source	Fuel	Blend	Density	C [%m/m]	FC_{vol} [%change]	CO_2 [%change]
4	HVO	100	780,3	84,61	1,39	-0,02
5	RME	30	853	83,4	2,04	-1,27
5	HVO	30	812,2	85,4	0,71	-0,23
6	GTL	100	774	84,82	0,54	-1,00
8	Hck/HVO	70/30	822,3	86	-2,88	-3,11
10	RME	100	876	77,07	7,78	-3,63

Table 16: Comparison of CO_2 emissions for different fuels based on fuel consumption values obtained from the model.

6 Conclusions

Results from the thesis give a new insight on engine performance with respect to fuel properties. The outcomes predict a final performance of passenger car from the end-user point of view. Modeling is based on extensive literature review and data collected from publicly available sources. Inconsistency in nomenclature and non-representative test set-ups were main initial obstacles while approaching the task of ADVANCEFUEL project. Problematic was a contradiction of some results in the literature and many reviews indicated discrepancies in terms of BSFC or BTE for similar fuel blends. In order to make a database, there was a need for extraction of data from different sources such as articles, publications and journal papers. However, the researches were done on miscellaneous engines, including small and big ones, also with changeable configuration characterized by the number of cylinders, total displacement, compression ratio. For that reason, the measurements were not always reflecting real driving conditions in a good way and a lot of data was rejected from modeling purposes. Moreover, it was hard to compare the final results, even though the aims of researches were the same. Nevertheless, combining multiple sources was essential for creating a model. Another important observation was a fact that standard diesel varies a lot when analyzing batches from different parts of the globe. Final properties are dependent on an origin of crude oil, refinement process and blending practices. The same situation applies to fuel blends, which express different final properties, although blending ratio is the same. All above conclusions from literature revealed the complexity of the problem while comparing results from various sources. ADVANCEFUEL project was aiming at the examination of alternative fuels with near future potential. In order to accomplish this task, proposed fuel should be compatible with current infrastructure. In this work, main attention was paid to drop-in fuels, which can be used directly in existing engines and are quite well tested. The work encompassed such fuels as traditional biodiesel (FAME), hydrotreated vegetable oil (HVO) and biomass-to-liquid (BTL) diesel. HVO and BTL are paraffinic high cetane number fuels, which are very promising replacements for standard fossil-based diesel. They own significantly better performance in modern engines than traditional biodiesel (FAME) and seem to prevail in the near future, providing that sustainability requirement is fulfilled.

In a majority of available sources, steady state measurements were conducted. Besides fuel and its properties, engine performance is also dependent on load, speed or driving conditions in general. Type of engine has an impact, too. It is clearly apparent when results from different experimental set-ups are compared. That is confirmed by the tests done with a use of RME in various researches. In articles 'A', 'B', 'C', 'D' described in Section 4.4, discrepancies between the outcomes are observed. Even though the engine operating conditions are similar and volumetric concentration of RME is the same, significant divergence in brake specific fuel consumption is evident. For example, the relative change of BSFC is in a range from 0 to +10% for 20% blend (B20 fuel). In article 'B' the BSFC slightly increases while in source 'A' significant growth is observed. Moreover, in paper 'D' there is some non-linear behavior noticed - for 10% blend, the BSFC is the lowest and in higher concentrations, it rapidly increases. Variations in brake thermal efficiency are even more apparent. In source 'B' with an increase of blending ratio, the growth of BTE is observed. In contrary, for source 'A' significant drop is monitored, whereas for source 'C' almost no changes are reported. For research 'D' there is a peculiar behavior for low blending ratios. From such a database created from the combination of previous articles, it is not possible to extract some universal behavior, even for one specified alternative fuel blend. Consequently, it is not feasible to use aforementioned data for modeling purposes.

Alternatively, steady state measurements can be analyzed for completely different renewable fuels on the same engine. Based on data from IEA AMF project, it was possible to present the impact of HVO, FAME and enzymatic FAME on the final performance of modern EURO VI engine in comparison with standard diesel fuel. Pure alternatives were tested in a wide range of operating conditions specified by load and speed of an engine. It turned out that working conditions have a huge impact on how fuel properties affect engine performance. In a case of HVO, fuel consumption for idling mode is slightly increased (+2%) when compared to standard diesel. The opposite effect is observed for high speed and high load (-5%). Moreover, for moderate operating conditions significant reductions in fuel consumption are observed (up to -9%). For enzymatic biodiesel (E-FAME), fuel consumption is higher in all cases but the extreme values range from 9,5% to 14,5%. For standard FAME, BSFC is increased only 8% for $50Nm/1500rpm$ steady state while 20% growth is noticed for $20Nm/1000rpm$. Not only BSFC is highly dependent on operational conditions, also other parameters are affected, i.e. NO_x emissions. Therefore, it is apparent that despite having data from measurements in full spectrum of engine's operational conditions, it is still not guaranteed to draw any general conclusions. Hence, the new methodology should be applied when examining an impact of fuel and its properties from the end-user point of view.

Driving cycle procedures are an optional way for analysis. They are weighted average from steady states and can mitigate the influence of the engine on final performance. Moreover, during real driving, there are many transient conditions, which cannot be represented by steady state operation. From the end-user point of view, NEDC or WLTC are better reflecting reality when considering passenger cars. Especially, measurements done on modern vehicles present in the market are much more valuable for modeling process. Test engine specifications are very significant and more reliable are runs on the representative engine instead of non-commercial set-up. In addition, the modeling process can only give such an outcome, which corresponds to the collected input information. Data for modeling should be always carefully selected in order to provide adequate model quality. It is the reason behind rejecting 3 sources of initial 10 with driving cycle test procedures described in Section 4.5. The ultimate sources used for modeling are the latest articles with researches conducted on representative engines during NEDC or WLTC cycles. Such a careful selection makes the results more reliable and promising.

Very important stage of the thesis encompassed identification of the most prominent properties influencing fuel consumption. For modeling purposes, 5 properties were selected: LHV, cetane number, density, viscosity, density and oxygen content. It was decided to choose volumetric lower heating value as a parameter reflecting the amount of fuel handled by injection system. Cetane number was chosen as the main parameter responsible for ignition quality. Density, viscosity and oxygen content were identified to be the most influential on injection, mixing and combustion process in a diesel engine. Additionally, the carbon content was the sixth parameter used for calculation of CO_2 emissions based on carbon balance. Another major step was related to relative changes approach, which enabled to combine different sources and compare results. After visualization of alternative fuel properties impact on fuel consumption, some trends in behavior were revealed, i.e. the linear relationship between LHV and fuel consumption. Moreover, based on results from available literature sources, it turned out that there is a directly proportional correlation between volumetric LHV and fuel consumption. Linear regression confirmed that the lower LHV is, the more fuel is needed and a slope of the fitting is very close to *-1*.

Final outcomes of modeling work are presented in Section 5.2. Applied multilinear regression resulted in Equation 5.2.1. The purpose of this relation is to predict fuel consumption based only on final properties of the fuel blend. The overall quality of fitting can be estimated by adjusted R-square, which is equal 0,917. Taking into account that model is universal for completely different types of fuels including HVO and FAME, the outcome is satisfactory. Moreover, standard errors of coefficients are in allowed range. That is why model estimates performance with fairly good accuracy. Cross-validation, executed while excluding one literature source, revealed that coefficients do not deviate too much. An important conclusion can be drawn from the data used for multilinear regression procedure. Although fuel blends have the same concentration of an alternative component, differences in fuel consumption can be noticed when comparing various literature results. It is caused by final fuel blend specification - concentration is the same but final properties are different. The model takes it into account and validation for various fuels is presented in Table 12. Based on Equation 5.2.1, the contribution of a single property on BSFC can be associated with the corresponding coefficient used in the final formula. Table 13 demonstrates how single property impacts fuel consumption while other properties are kept constant. Extreme allowable changes are taken into account and they are associated with pure alternative fuels' property deviations from standard diesel. The biggest impact owns LHV, which directly and proportionally influences BSFC. The highest growth in FC is reported for a biodiesel-like blend, up to 15%. Moreover, the higher the cetane number is, the lower FC is noticed - reduction over 4% can be reached. For density and oxygen content proportional relation is observed, in contrary to viscosity. However, those properties increase at maximum FC below 2%. Two counteracting effects are explaining moderate influence of oxygen content. On the one hand, it improves the combustion characteristic but on the other hand, it lowers the calorific value of the fuel. Additionally, pure DME fuel was tested on the model. Despite it is not a drop-in fuel and normally in gaseous form, the results are promising. Worth mentioning is a fact that during injection DME is in liquid form and thus the nature of combustion is similar to standard diesel. The model indicates a significant increase in fuel consumption around 48,7%, what is consistent with expectations. Finally, CO_2 emissions are based on carbon balance. The results of fuel consumption are directly used to predict CO_2 emissions. For specified fuel blends, it is important to know carbon content in pure fuels. The outcomes for various blends are collected in Table 16. Highest reductions are observed for RME. However, those are only tailpipe emissions. In order to assess the sustainability of a fuel, complete WTW analysis should be performed.

6.1 Limitations and future recommendations

The model proposed in the thesis estimates light-duty engine performance in terms of fuel consumption and emissions. The main aim is to predict how changes of final fuel blend properties will influence fuel consumption and emissions. However, the results of the modeling work are based on multiple literature sources with different experimental set-ups. The outcomes are very sensitive to the data provided for analysis. In order to further validate the correctness of the model, it would be very beneficial to use data from a commercial sector, i.e. from one of the stakeholders. Such a new database with no doubt would contribute to improvements of the model.

Analyzing only few fuel types, it is obvious that properties are interconnected. One option to examine the impact of the single property would be an analysis of triple blends. Even more component blends could be used, following refinery practices. The main research would require keeping some properties constant while changing others. Some trials were performed already and can be found in the literature. For example, either oxygen content or cetane number can be kept constant, as in [68] and [69]. In another research ([70]) multiple oxygenates samples are tested and emissions analyzed.

For the purpose of ADVANCEFUEL project, there is a special attention paid to second generation biofuels, such as BTL produced from cellulosic feedstock. However, the results for BTL performance are rarely published. In the model, multiple samples with BTL fuel should be included in order to more accurately predict the performance of similar fuels. Next step of research could be also related to the analysis of optimized engines, with specially adjusted ECU for alternative fuel purposes. HVO could be used in dedicated engines and it would positively affect the efficiency of a diesel engine. Then more gains could be observed, including decreased fuel consumption and lower emission levels.

Certainly, there is a need for new models in other transportation sectors such as aviation, marine. In those modes, steady state conditions are prevailing and slightly different approach should be applied. The outcomes of this thesis are very promising and work should be continued in reference to ADVANCEFUEL project and beyond.

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A Appendix A

Compression Ignition Engine fuels	Property			CN	Density	LHV	LHV vol	Viscosity	C	H	O
	Unit			-	kg/m3 @15 C	MJ/kg	MJ/l	mm2/s @40 C	% m/m	% m/m	% m/m
	Standard diesel	Germany	Typical diesel	53,5	830,0	42,80	35,52	2,6	85,8	13,49	0,72 (5-7% FAME)
		USA	Chevron	44,7	843,8	42,60	35,95	2,24	87,14	12,86	0
		Finland	Neste Futura (-5/-15)	54,0	825,0	43,28	35,71	3,00	86,2	13,8	0 (0% FAME)
			Neste Pro (15% v/v HVO)	60,0	826,0	43,28	35,75	3,00	86,2	13,8	0 (0% FAME)
			St1 Diesel plus -20	63,0	805,0	43,28	34,84	3,10	n.d.	n.d.	0,2 (1,5% FAME)
	FAME	Animal	Beef tallow	60,9	874,3	37,22	32,54	4,83	76,09	12,60	11,35
			Fish	51,0	887,3	38,80	34,43	4,30	77,40	11,85	10,75
			Palm	61,2	874,7	37,08	32,43	4,61	76,09	12,44	11,27
		EU	Rapeseed	54,1	882,2	37,63	33,20	4,63	77,07	11,84	10,93
		US	Soybean	51,8	882,8	37,75	33,33	4,29	77,03	11,90	10,95
		Waste	WCO	56,2	880,6	37,88	33,36	4,75	76,90	12,02	10,77
	HVO		Neste Renewable Diesel (I)	88,0	780,0	44,10	34,40	2,87	84,61	14,67	0,00
			Neste HVO (II)	80,0	780,3	43,60	34,02	2,87	84,61	14,67	0,00
			Neste HVO (III)	94,8	780,0	43,95	34,28	2,99	84,68	14,52	0,00
			HVO - Universal Oil Products	81,8	775,8	43,86	34,03	2,65	84,84	15,16	0,00
	GTL/BTL		SunDiesel BTL CHOREN 2005	80,0	761,2	44,58	33,93	1,55	85,79	12,54	1,67
			FT fuel as GTL	81,2	770,0	43,70	33,65	2,79	84,94	15,06	0,00
			Shell GTL (I) - FT from NG	80,0	784,6	43,90	34,44	3,50	85,00	15,00	0,00
			Shell GTL (II)	75,4	777,0	43,58	33,86	3,13	85,85	14,15	0,00
			Shell GTL (III)	75,0	776,9	43,25	33,60	2,53	85,83	14,17	0,00
			Shell GTL (IV)	75,0	779,0	43,60	33,96	2,74	84,90	15,10	0,00
			SASOL GTL FT diesel	89,2	774,0	44,03	34,08	2,34	84,82	15,18	0,00
	DME		IEA AMF data collected	57,5	660,0	28,00	18,48	below 1	52,00	13,00	35,00
	SVO		Neat rapeseed oil	39,0	920,0	37,10	34,13	35,00	78,00	13,50	8,90
	Ethanol		Pure ethanol	8,0	788,0	26,80	21,12	1,20	52,17	13,04	34,78

Figure A1: CI engine fuels - property table based on [26], [27], [28], [35], [36], [53], [56], [57], [71], [72], [73], [74], [75], [76], [77], [78].